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Chapter 1 - Wave propagation and interaction with the sample

PHYS-715 Physical Optics and Advanced Imaging 2024

Course contents

Cover the unifying concepts of imaging, including with electrons, optics, X-rays. In 2D, 3D, and beyond.

Chapter 1 Interactions of waves with the sample and beyond

- Review of Fourier transform and properties
- Helmholtz equation
- Angular spectrum and evanescent waves
- Huygens–Fresnel principle
- Rayleigh-Sommerfeld solution
- Fresnel approximation
- Fraunhofer approximation – the far field
- Paraxial wave equation
- Projection approximation
- Multislice propagation
- Beer-Lambert law

Review of Fourier transform and properties

The Fourier transform (FT)

FT is a mathematical transform. From "real" space to "reciprocal" or "frequency" space

Very common in the time domain → can be understood as frequencies

"Physical possibility is a valid sufficient condition for the existence of a transform" [1]

e.g. Finite energy

$$G(f) = \mathcal{F}\{g(t)\} = \int_{-\infty}^{\infty} g(t)e^{-i2\pi(ft)}dt$$

$$g(t) = \mathcal{F}^{-1}\{G(f)\} = \int_{-\infty}^{\infty} G(f)e^{i2\pi(ft)}dt$$

We will use here the symmetric definition in terms of frequencies (revolutions per second).
Other definitions in terms of angular frequency (radians per second) can be symmetric or not symmetric.

[1] R.N. Bracewell. The Fourier Transform and Its Applications. McGraw-Hill Book Company, Inc., New York, second revised edition, 1965.

The Fourier transform (FT)

FT for each frequency, is a projection unto an oscillatory kernel, which quantifies how much of that frequency is present in the signal

It is a decomposition of g into a linear combination of oscillatory elementary functions. G is namely the coefficient for that elementary function.

Any function in time that exists can be expanded into a sum of sines and cosines

$$G(f) = \mathcal{F}\{g(t)\} = \int_{-\infty}^{\infty} g(t) e^{-i2\pi(ft)} dt$$

$$g(t) = \mathcal{F}^{-1}\{G(f)\} = \int_{-\infty}^{\infty} G(f) e^{i2\pi(ft)} dt$$

$$e^{-i2\pi(ft)} = \cos(2\pi f t) - i\sin(2\pi f t)$$

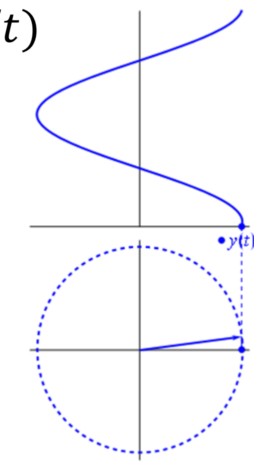

Image from https://en.wikipedia.org/wiki/Fourier_transform

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$$G(f) = \mathcal{F}\{g(t)\} = \int_{-\infty}^{\infty} g(t) e^{-i2\pi(ft)} dt$$

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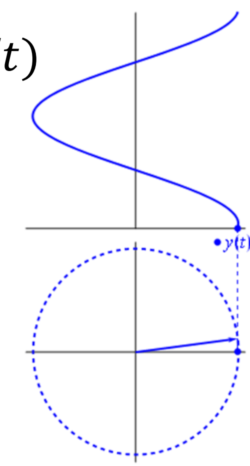


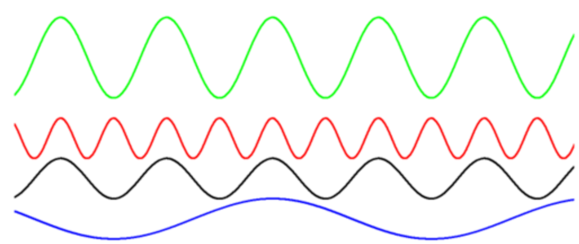


Image from https://en.wikipedia.org/wiki/Fourier_transform
Image from https://www.ck12.org/trigonometry/period-and-frequency/lesson/Frequency-and-Period-of-Sinusoidal-Functions-PCALC/

The 2D spatial Fourier transform

Why? <u>Its very useful</u>

→ A sine wave is a good basis to solve linear wave phenomena → If you solve for one wave you solve for anything

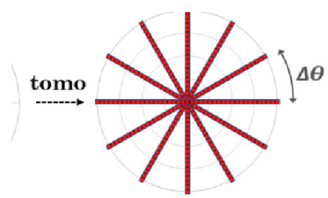
→ Optics response

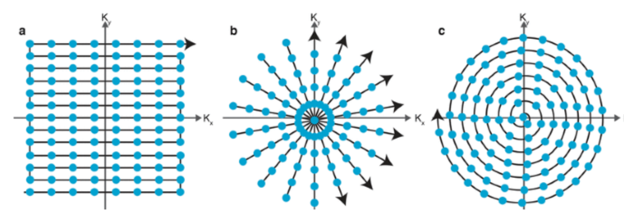
→ Propagation to far field

→ Image processing

→ Tomography, MRI, can be studied in Fourier domain

M100 images taken before and after a 1993 space shuttle repair mission to correct Hubble's flawed optics. Image: NASA, ESA

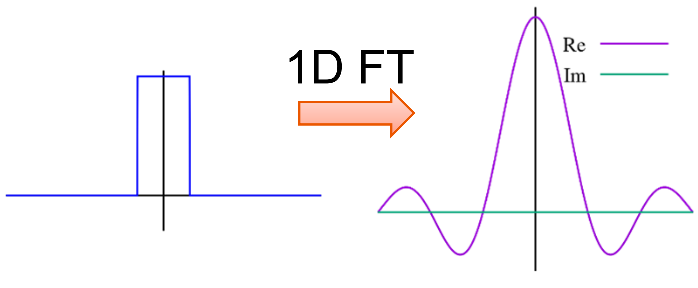


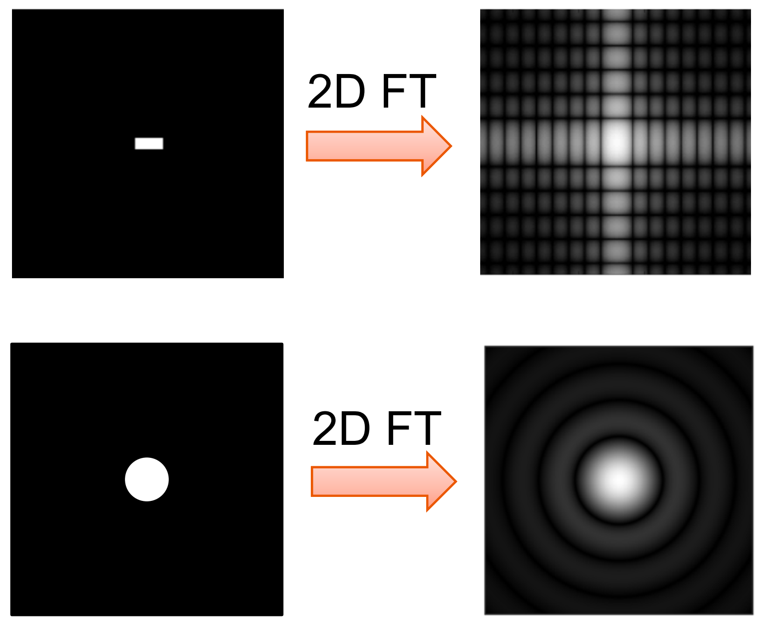


Basic Principles of Cardiovascular MRI, Springer 2015

The 2D Fourier transform

The 2D FT is very important concept in optics, imaging, and tomography. It is a straightforward generalization of the 1D FT.





Images from https://en.wikipedia.org/ and https://www.chegg.com

The 2D spatial Fourier transform

A particular spatial frequency is associated with a period in space

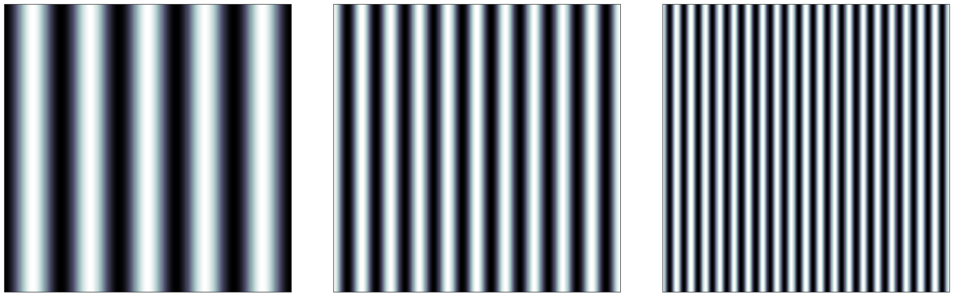
→ units are cycles/meter

$$f_x = \frac{1}{\tau_x}$$

$$G(f_x, f_y) = \mathcal{F}\{g(x,y)\} = \iint_{-\infty}^{\infty} g(x,y) e^{-i2\pi(f_x x + f_y y)} dx dy$$

$$g(x,y) = \mathcal{F}^{-1}\{G(f_x, f_y)\} = \iint_{-\infty}^{\infty} G(f_x, f_y) e^{i2\pi(f_x x + f_y y)} df_x df_y$$

Example of fx with different values



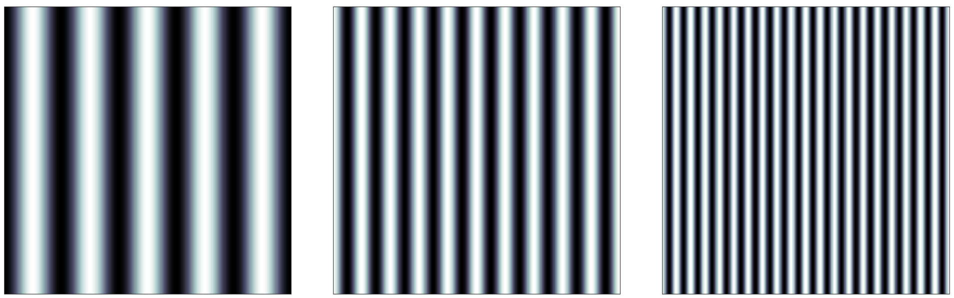
$f_x = 5, 10, 20$ ${}^{\text{cycles}}/_{\text{m}}$

$f_y = 0, 0, 0$ ${}^{\text{cycles}}/_{\text{m}}$

What happens if I have then non-zero f_y?

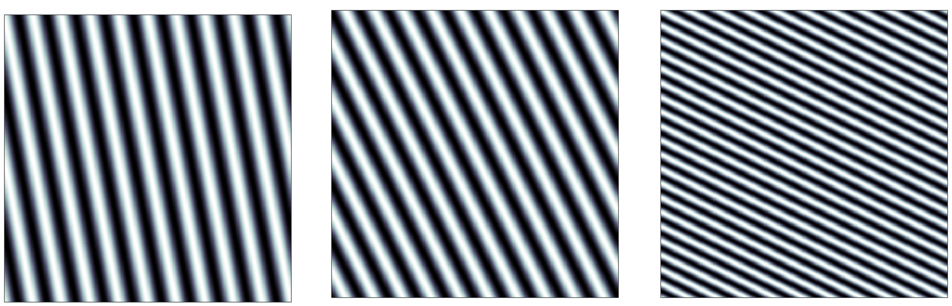
Basis functions of the 2D FT

$\cos(2\pi[f_x x + f_y y])$



$f_x = 5, 10, 20 \ \text{cycles}/\text{m}$

$f_y = 0, 0, 0 \ \text{cycles}/\text{m}$



$f_x = 10, 10, 10 \ \text{cycles}/\text{m}$

$f_y = 2, 5, 20 \ \text{cycles}/\text{m}$

spatial_frequency.m

Theorems of the FT

Dirac delta (not a theorem)	$\mathcal{F}\{1\} = \delta(f_x, f_x)$
Separability	$\mathcal{F}\{g(x)h(y)\} = \mathcal{F}_{1D}\{g(x)\}\mathcal{F}_{1D}\{h(y)\}$
Linearity	$\mathcal{F}\{ag(x,y) + bh(x,y)\} = a\mathcal{F}\{g(x,y)\} + b\mathcal{F}\{h(x,y)\}$
Similarity (scaling)	$\mathcal{F}\{g(ax,by)\} = \frac{1}{\lvert ab\rvert} G\left(\frac{f_x}{a}, \frac{f_y}{b}\right)$
Shift	$\mathcal{F}\{g(x-a, y-b)\} = G(f_x, f_y)\exp(-i2\pi[f_x a + f_y b])$
Rayleigh's theorem (Parseval's)	$\iint_{-\infty}^{\infty} \lvert g(x,y)\rvert^2 dxdy = \iint_{-\infty}^{\infty} \lvert G(f_x, f_y)\rvert^2 df_x df_y$

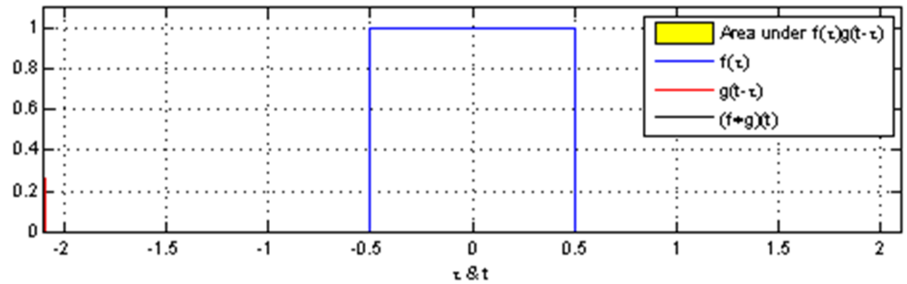
J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)

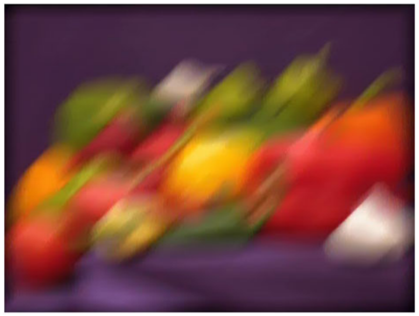
Theorems of the FT

Convolution $$g(x,y) * h(x,y) = \iint_{-\infty}^{\infty} g(\xi,\eta)h(x-\xi,y-\eta)d\xi d\eta$$

$$\mathcal{F}\{g(x,y) * h(x,y)\} = G(f_x,f_y)H(f_x,f_y)$$

Sifting property $$g(x,y) * \delta(x-a,y-b) = g\,(x-a,y-b)$$





J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)
https://en.wikipedia.org/wiki/Convolution#/media/File:Convolution_of_box_signal_with_itself2.gif
Matlab "imfilter.m" documentation

Theorems of the FT

Autocorrelation $\mathcal{F}\{|g(x,y)|^2\} = G(f_x, f_y) * G^*(-f_x, -f_y) = G(f_x, f_y) \star G(f_x, f_y)$

Rotation $\mathcal{F}\{\mathrm{R}_\theta\{g(x,y)\}\} = \mathrm{R}_\theta\{G(f_x, f_y)\}$

Successive transform $\mathcal{F}\{\mathcal{F}\{g(x,y)\}\} = g(-x,-y)$

J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)

Fourier transform pairs

Table 2.1: Transform pairs for some functions separable in rectangular coordinates.

Function	Transform
$\exp[-\pi(a^2x^2+b^2y^2)]$	$\frac{1}{\lvert ab\rvert}\exp\left[-\pi\left(\frac{f_X^2}{a^2}+\frac{f_Y^2}{b^2}\right)\right]$
$\mathrm{rect}(ax)\,\mathrm{rect}(by)$	$\frac{1}{\lvert ab\rvert}\mathrm{sinc}(f_X/a)\,\mathrm{sinc}(f_Y/b)$
$\Lambda(ax)\,\Lambda(by)$	$\frac{1}{\lvert ab\rvert}\mathrm{sinc}^2(f_X/a)\,\mathrm{sinc}^2(f_Y/b)$
$\delta(ax, by)$	$\frac{1}{\lvert ab\rvert}$
$\exp[j\pi(ax+by)]$	$\delta(f_X - a/2, f_Y - b/2)$
$\mathrm{sgn}(ax)\,\mathrm{sgn}(by)$	$\frac{ab}{\lvert ab\rvert}\frac{1}{j\pi f_X}\frac{1}{j\pi f_Y}$
$\mathrm{comb}(ax)\,\mathrm{comb}(by)$	$\frac{1}{\lvert ab\rvert}\mathrm{comb}(f_X/a)\,\mathrm{comb}(f_Y/b)$
$\exp[j\pi(a^2x^2+b^2y^2)]$	$\frac{j}{\lvert ab\rvert}\exp\left[-j\pi\left(\frac{f_X^2}{a^2}+\frac{f_Y^2}{b^2}\right)\right]$
$\exp[-(a\lvert x\rvert+b\lvert y\rvert)]$	$\frac{1}{ab}\frac{2}{1+(2\pi f_X/a)^2}\frac{2}{1+(2\pi f_Y/b)^2}$

$(a > 0, b > 0)$

J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)

FFT camera

Live examples with FFT camera

Exercises

Instructions for online students:

- Download the FFTcamera app
- Download from moodle or course page “FFTcamera material.pptx”
- Follow the instructions in the notes of the slides

Lecture 2

Any questions about previous lecture?

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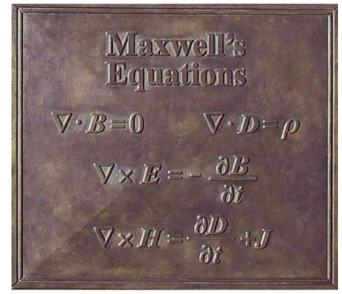
Helmholtz equation

Maxwell's equations – Differential form

Represent the state of electromagnetic theory on the 1800s



Edinburgh

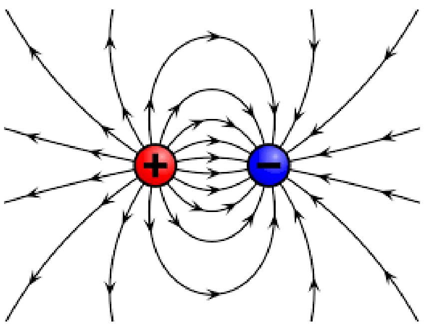
James C. Maxwell
(1831 – 1879)

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

Gauss's law

Divergence of electric fields is non-zero only if there are charges

Electric fields begin and end in a charge



$$\nabla = \frac{\partial}{\partial x}\hat{i} + \frac{1}{\partial y}\hat{j} + \frac{1}{\partial z}\hat{k}$$

$$\nabla \cdot \mathbf{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z}$$

$\mathbf{E} \rightarrow$ Electric field

$\mathbf{B} \rightarrow$ Magnetic field

$\rho \rightarrow$ Electric charge density

$\varepsilon_0 \rightarrow$ Permitivity of free space

$\mu_0 \rightarrow$ Permeability of free space

D. J. Griffiths, Introduction to electrodynamics, third edition. Prentice Hall (1999)
https://en.wikipedia.org/wiki/History_of_Maxwell%27s_equations
https://en.wikipedia.org/wiki/Maxwell%27s_equations

Maxwell's equations – Differential form

Represent the state of electromagnetic theory on the 1800s

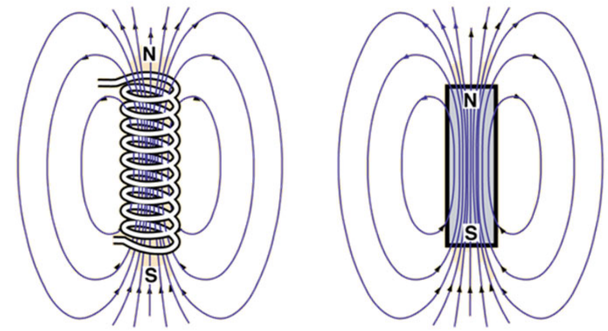
$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

<u>Gauss's law</u>
Divergence of electric fields is non-zero only if there are charges
Electric fields begin and end in a charge

$$\nabla \cdot \mathbf{B} = 0$$

Divergence of magnetic field is always zero
There are no magnetic charges, or monopoles

D. J. Griffiths, Introduction to electrodynamics, third edition. Prentice Hall (1999)
https://en.wikipedia.org/wiki/History_of_Maxwell%27s_equations
https://en.wikipedia.org/wiki/Maxwell%27s_equations



http://hyperphysics.phy-astr.gsu.edu/hbase/magnetic/elemag.html#c1

$$\nabla = \frac{\partial}{\partial x}\hat{i} + \frac{1}{\partial y}\hat{j} + \frac{1}{\partial z}\hat{k}$$

$$\nabla \cdot \mathbf{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z}$$

$\mathbf{E} \rightarrow$ Electric field

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Maxwell's equations – Differential form

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

Faraday's law (Induction)

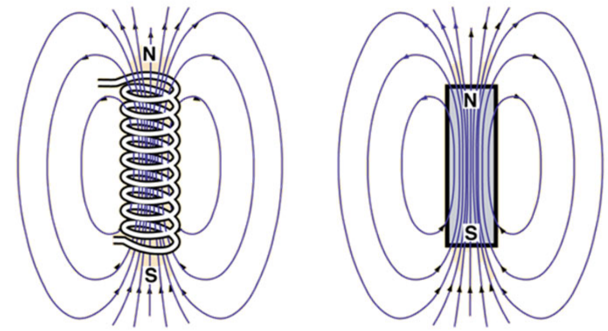
A time varying magnetic field always comes with a spatially variant electric field.

Transformers, inductors, electric motors, generators…

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

Ampere-Maxwell law

A current creates a circulating magnetic field. Also a time-varying electric field.



http://hyperphysics.phy-astr.gsu.edu/hbase/magnetic/elemag.html#c1

$$\nabla = \frac{\partial}{\partial x}\hat{i} + \frac{1}{\partial y}\hat{j} + \frac{1}{\partial z}\hat{k}$$

$$\nabla \cdot \mathbf{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z}$$

$\mathbf{E} \rightarrow$ Electric field

$\mathbf{B} \rightarrow$ Magnetic field

$\mathbf{J} \rightarrow$ Current density

$\rho \rightarrow$ Electric charge density

$\varepsilon_0 \rightarrow$ Permitivity of free space

$\mu_0 \rightarrow$ Permeability of free space

D. J. Griffiths, Introduction to electrodynamics, third edition. Prentice Hall (1999)
https://en.wikipedia.org/wiki/History_of_Maxwell%27s_equations
https://en.wikipedia.org/wiki/Maxwell%27s_equations

Electromagnetic waves

Assuming vacuum and no sources we can combine the four equations into wave equations for **E** and **B**

$$\nabla \cdot \mathbf{E} = 0 \qquad \nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \times \mathbf{B} = \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

$$\nabla^2 \mathbf{E} = \mu_0 \varepsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2} \qquad \nabla^2 \mathbf{B} = \mu_0 \varepsilon_0 \frac{\partial^2 \mathbf{B}}{\partial t^2}$$

If the different directions of polarization do not interact then we arrive at a scalar wave equation

$$\nabla^2 E = \mu_0 \varepsilon_0 \frac{\partial^2 E}{\partial t^2} = \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2}$$

$$\nabla = \frac{\partial}{\partial x}\hat{i} + \frac{1}{\partial y}\hat{j} + \frac{1}{\partial z}\hat{k}$$

$$\nabla^2 \mathbf{E} = \nabla^2 E_x \hat{i} + \nabla^2 E_y \hat{j} + \nabla^2 E_z \hat{k}$$

$$\nabla^2 E_x = \frac{\partial^2 E_x}{\partial^2 x} + \frac{\partial^2 E_x}{\partial^2 y} + \frac{\partial^2 E_x}{\partial^2 z}$$

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https://en.wikipedia.org/wiki/Maxwell%27s_equations

Electromagnetic waves

Maxwell's equations imply that there is such thing as electro-magnetic waves

They propagate in vacuum

Speed happens to be equal to the speed of light

Is light an electromagnetic wave that can propagate in vacuum?

"We can scarcely avoid the inference that light consists in the transverse undulations of the same medium which is the cause of electric and magnetic phenomena"

$$\nabla^2 E = \mu_0 \varepsilon_0 \frac{\partial^2 E}{\partial t^2} = \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2}$$

In polarizable matter a small modification can be made to account for only «free charges» and local polarization

$$\nabla^2 E = \mu \varepsilon \frac{\partial^2 E}{\partial t^2} = \frac{n^2}{c^2} \frac{\partial^2 E}{\partial t^2}$$

$$\nabla = \frac{\partial}{\partial x}\hat{i} + \frac{1}{\partial y}\hat{j} + \frac{1}{\partial z}\hat{k}$$

$$\nabla^2 \mathbf{E} = \nabla^2 E_x \hat{i} + \nabla^2 E_y \hat{j} + \nabla^2 E_z \hat{k}$$

$$\nabla^2 E_x = \frac{\partial^2 E_x}{\partial^2 x} + \frac{\partial^2 E_x}{\partial^2 y} + \frac{\partial^2 E_x}{\partial^2 z}$$

D. J. Griffiths, Introduction to electrodynamics, third edition. Prentice Hall (1999)

Monochromatic waves

Any electric field can be expressed as a superposition of different frequencies. We can solve the equation for one frequency at a time

$$E(\mathbf{r},t) = \int_{-\infty}^{\infty} \tilde{E}(\mathbf{r},\omega)\exp(-i\omega t)\,d\omega$$

$$\nabla^2 E = \frac{n^2}{c^2}\frac{\partial^2 E}{\partial t^2} \qquad \nabla^2 \tilde{E}(\mathbf{r},\omega) = -\frac{\omega^2 n^2(\mathbf{r},\omega)}{c^2}\tilde{E}(\mathbf{r},\omega)$$

$$\nabla^2 \tilde{E}(\mathbf{r},\omega) + k_0{}^2 n^2(\mathbf{r},\omega)\tilde{E}(\mathbf{r},\omega) = 0$$ Scalar Helmholtz equation

$$k_0 = \frac{\omega}{c} \qquad k_0 = \frac{2\pi}{\lambda_0} \qquad \omega = 2\pi f$$

- $k_0 \rightarrow$ Wavenumber in free space
- $\lambda_0 \rightarrow$ Wavelength in free space
- $\omega \rightarrow$ Angular frequency
- $f \rightarrow$ Frequency

Helmholtz equation

$$\nabla^2 \tilde{E}(\mathbf{r},\omega) + {k_0}^2 n^2(\mathbf{r},\omega)\tilde{E}(\mathbf{r},\omega) = 0$$

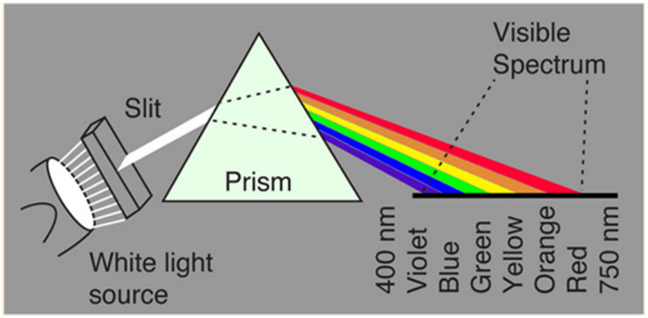
$$E(\mathbf{r},t) = \mathrm{Re}\{\tilde{E}(\mathbf{r},\omega)\exp(-i\omega t)\}$$

Solution gives a description of interaction of wave and sample

Electric fields are real, for linear systems we can use phasors as a mathematical convenient shortcut

Index of refraction depends on space (sample geometry) and frequency (dispersion)

This dependance allows us to use EM waves to extract information from the materials

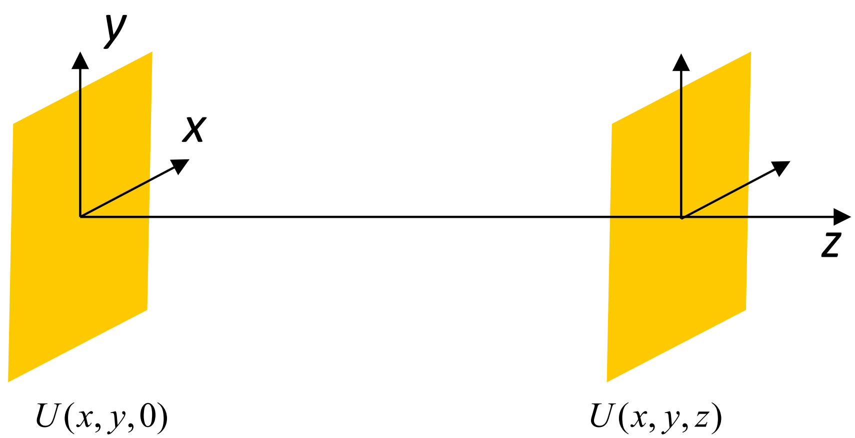


http://hyperphysics.phy-astr.gsu.edu/hbase/geoopt/dispersion.html

Free space propagation – Angular spectrum

Propagation calculation by angular spectrum

Goal: Predict field in plane (x, y, z) from field in plane (x, y, 0)



$$A(f_x, f_y; 0) = \mathcal{F}\{U(x, y, 0)\} = \iint_{-\infty}^{\infty} U(x, y, 0)\exp\left[-i2\pi(f_x x + f_y y)\right]dxdy$$

$$U(x, y, 0) = \mathcal{F}^{-1}\{A(f_x, f_y; 0)\} = \iint_{-\infty}^{\infty} A(f_x, f_y; 0)\exp\left[i2\pi(f_x x + f_y y)\right]df_x df_y$$

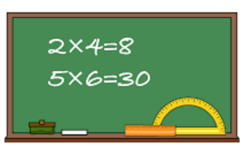
$$\nabla^2 U + k_0{}^2 U = 0$$

Propagation calculation by angular spectrum

We start with the Ansatz of a plane-wave as a solution of the Helmholz equation
an idealization of an infinite and perfectly flat wavefront

$$p(x, y, z) = \exp\left[i\mathbf{k} \cdot \mathbf{r}\right]$$

$$k_0^2 = \left(\frac{2\pi}{\lambda_0}\right)^2 = k_x^2 + k_y^2 + k_z^2$$



$$\nabla^2 U + k_0{}^2 U = 0$$

A is the angular spectrum of U
Why is it called that?

$$A\left(f_x, f_y; 0\right) = \mathcal{F}\left\{U\left(x, y, 0\right)\right\} = \iint_{-\infty}^{\infty} U\left(x, y, 0\right) \exp\left[-i2\pi(f_x x + f_y y)\right] dxdy$$

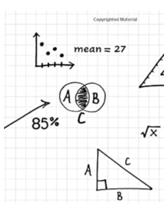
$$U\left(x, y, 0\right) = \mathcal{F}^{-1}\left\{A\left(f_x, f_y; 0\right)\right\} = \iint_{-\infty}^{\infty} A\left(f_x, f_y; 0\right) \exp\left[i2\pi(f_x x + f_y y)\right] df_x df_y$$

A corresponds to the 2D Fourier coefficients of U we can take one particular component

$$U_{example}\left(x, y, 0\right) = A\left(f_x, f_y; 0\right) \exp\left[i2\pi(f_x x + f_y y)\right]$$

This component needs a z dependance to propagate as plane-wave

$$U_{example}\left(x, y, z\right) = A\left(f_x, f_y; 0\right) \exp\left[i2\pi(f_x x + f_y y + f_z z)\right]$$



$$U_{example}\left(x, y, z\right) = A\left(f_x, f_y; 0\right) \exp\left[i2\pi(f_x x + f_y y)\right] \exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2 - f_x^2 - f_y^2}\right]$$

$$\nabla^2 U + k_0{}^2 U = 0$$
$$k_x = 2\pi f_x$$

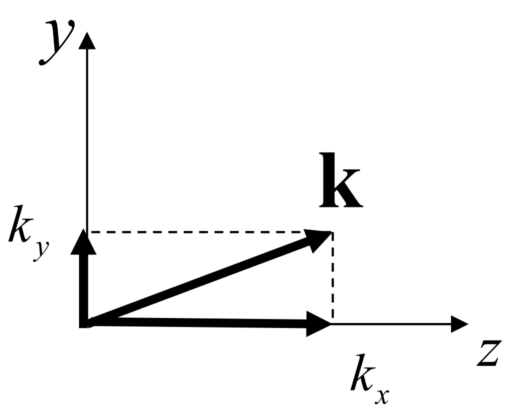
Prove that it satisfies Helmholtz equation!

A is the angular spectrum of U
Why is it called that?

$$U_{example}(x,y,z) = A\left(f_x, f_y; 0\right)\exp\left[i2\pi(f_x x + f_y y)\right]\exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2 - f_x^2 - f_y^2}\right]$$

$$U_{example}(x,y,z) = A\left(f_x, f_y; 0\right)\exp\left[i(k_x x + k_y y)\right]\exp\left[iz\sqrt{k_0{}^2 - k_x^2 - k_y^2}\right]$$

$$k_z = \sqrt{k_0{}^2 - k_x^2 - k_y^2}$$



Each of the coefficients A, corresponds to a different direction of propagation

wave_moving.ipynb

$$\nabla^2 U + k_0{}^2 U = 0$$

$$k_x = 2\pi f_x$$

Each coefficient gets a different phase shift as we increase the observation plane z

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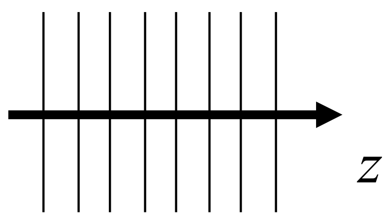
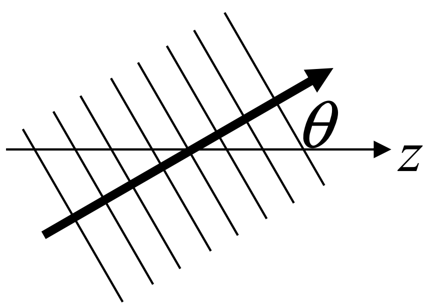
$$U_{example}(x,y,z) = A\left(f_x, f_y; 0\right)\exp\left[i2\pi(f_x x + f_y y)\right]\exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2 - f_x^2 - f_y^2}\right]$$



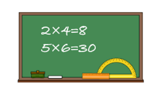
Accumulated phase shift is $f_x = 0, f_y = 0;$

$$\exp\left(ik_0 z\right)$$



Accumulated phase shift is $2\pi f_x = k_0 \sin\theta, \quad 2\pi f_y = 0, \quad 2\pi f_z = k_0 \cos\theta$

$$\exp\left(ik_0 z \cos\theta\right)$$



$$\nabla^2 U + k_0{}^2 U = 0$$

$$k_x = 2\pi f_x$$

By linearity

We add all of the propagated components

$$U(x,y,z)=\iint_{-\infty}^{\infty} A(f_x,f_y;0)\exp\left[i2\pi(f_x x+f_y y)\right]\exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2-f_x^2-f_y^2}\right]df_x df_y$$

$$U(x,y,z)=\iint_{-\infty}^{\infty} A(f_x,f_y;0)\exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2-f_x^2-f_y^2}\right]\exp\left[i2\pi(f_x x+f_y y)\right]df_x df_y$$

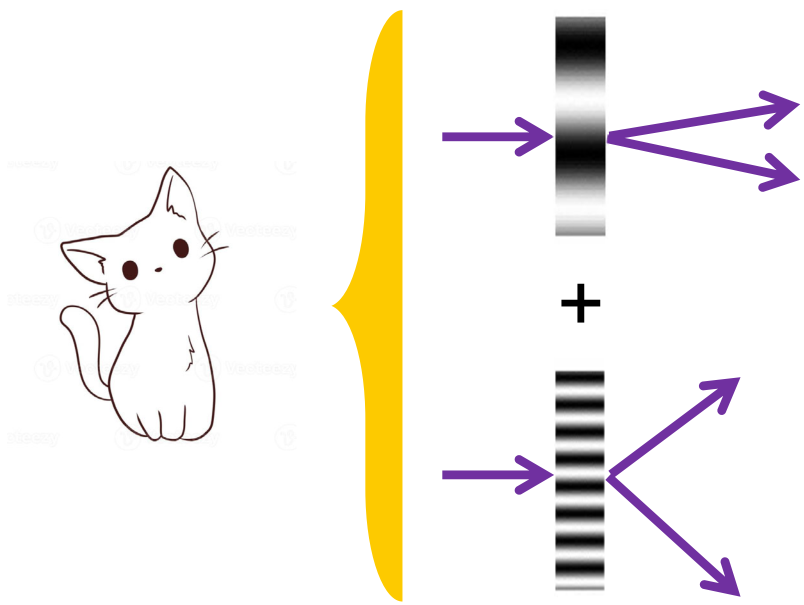
$$U(x,y,z)=\mathcal{F}^{-1}\left\{\mathcal{F}\{U(x,y,0)\}H(f_x,f_y)\right\}$$

$$H(f_x,f_y)=\exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2-f_x^2-f_y^2}\right]$$

Propagation is just a phase shift in Fourier domain

Decompose the input into plane-waves by FT, then propagate each one

Higher spatial frequencies of the object (resolution) propagate at higher angles



$$U(x,y,z)=\mathcal{F}^{-1}\left\{\mathcal{F}\left\{U(x,y,0)\right\}H(f_x,f_y)\right\}$$

$$H(f_x,f_y)=\exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2-f_x^2-f_y^2}\right]$$

Exact solution of Helmholtz equation

Evanescent waves

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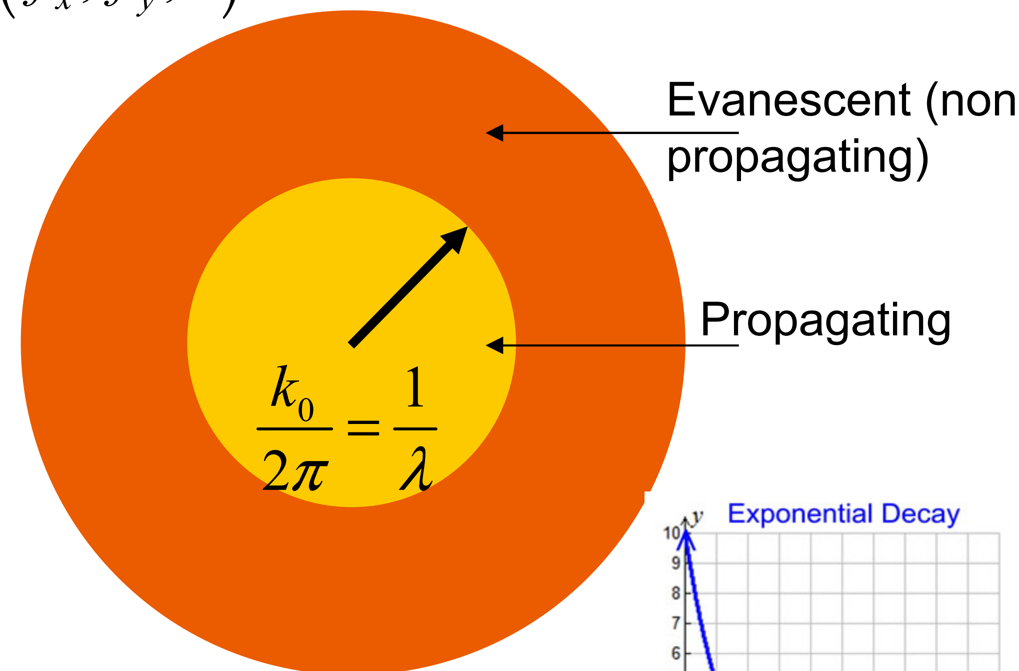
Evanescent waves

$$k_x^2 + k_y^2 > k_0^2$$

$$H(f_x, f_y) = \exp\left[i2\pi z \sqrt{\left(\frac{k_0}{2\pi}\right)^2 - f_x^2 - f_y^2} \right]$$

$$H(f_x, f_y) = \exp\left[-2\pi z \sqrt{f_x^2 + f_y^2 - \left(\frac{k_0}{2\pi}\right)^2} \right]$$

$$A(f_x, f_y; 0)$$



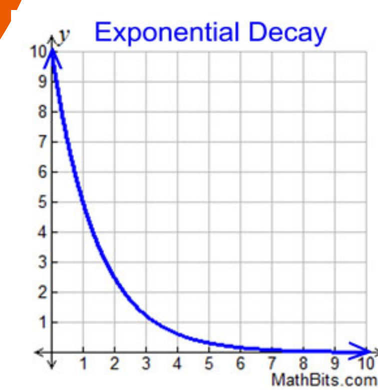


Image from https://mathbitsnotebook.com/Algebra1/Exponentials/EXGrowthDecay.html

Angular spectrum

Propagation as a linear spatial filter

Exact solution of scalar Helmholtz equation

Arbitrary angles of propagation

For linear systems it can be extended by linearity to

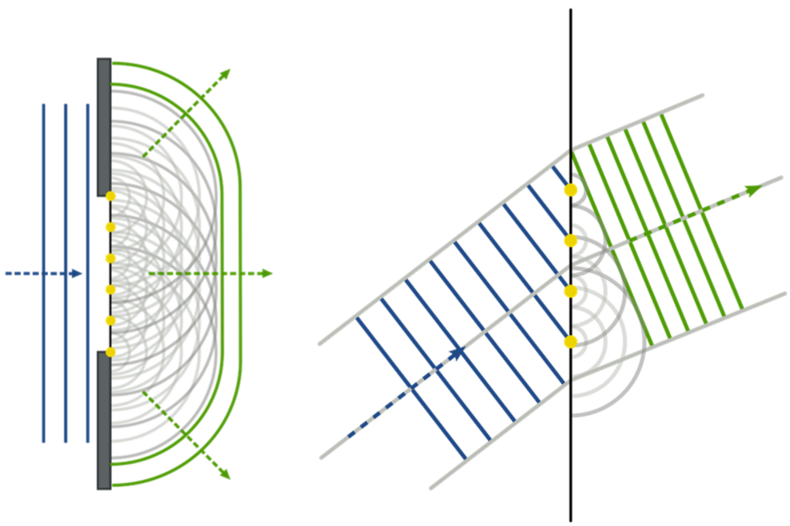
- Broadband light
- Vectorial light

Limitation: Only includes propagation in positive z direction

Huygens–Fresnel principle

Huygens-Fresnel principle

In 1678, Huygens proposed that every point reached by a luminous disturbance becomes a source of a spherical wave; the sum of these secondary waves determines the form of the wave at any subsequent time.



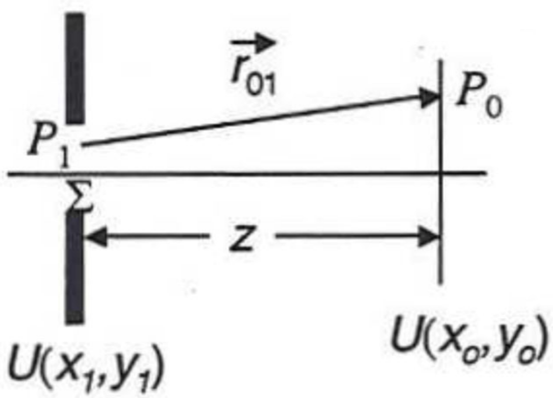
C. Huygens 1629-1695

A.-J. Fresnel 1788-1827

https://en.wikipedia.org/wiki/Huygens%E2%80%93Fresnel_principle

Huygens-Fresnel principle

Together with Fresnel's principle of interference this explained refraction and diffractive effects



$$U(P_0) = \frac{1}{i\lambda_0} \iint_{\Sigma_1} U(P_1) \frac{\exp(ikr_{01})}{r_{01}} ds_1$$

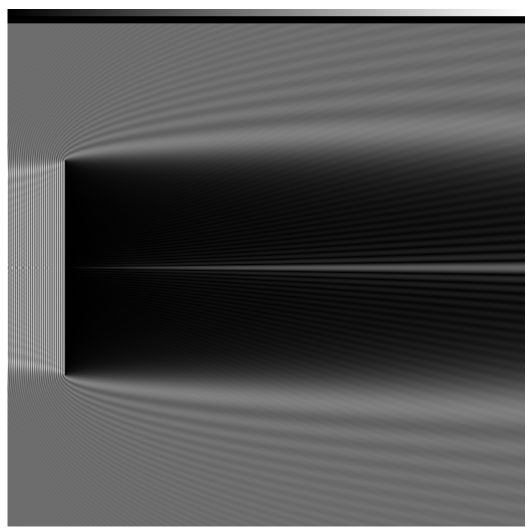
$$r_{01} = \sqrt{(x_0 - x_1)^2 + (y_0 - y_1)^2 + z^2}$$

The Poisson spot

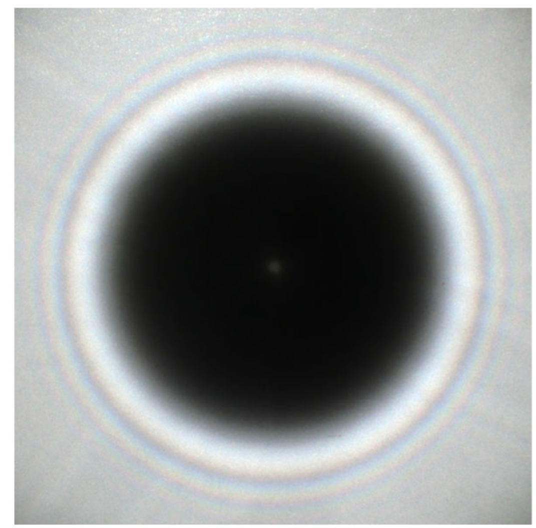
Poisson used Fresnel theory to predict that a bright spot would appear in the center of the shadow of a small disc → therefore the theory was incorrect

Arago performed the experiment which decidedly proved that light is a wave

Numerical simulation



Photo



https://en.wikipedia.org/wiki/Arago_spot

Does it satisfy the Helmholtz equation?

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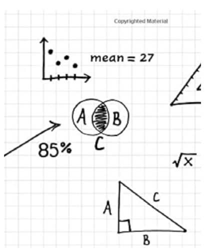
$$U\left(P_0\right)=\frac{1}{i\lambda_0}\frac{\exp\left(ikr_{01}\right)}{r_{01}}$$

$$r_{01}=\sqrt{(x_0-x_1)^2+(y_0-y_1)^2+z^2}$$

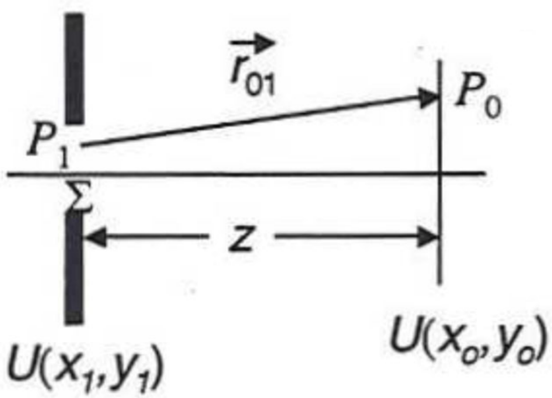


$$\nabla^2 U+k_0{}^2 U=0$$

Free space propagation – Rayleigh-Sommerfeld solution

Rayleigh-Sommerfeld solution

A solution can be obtained using Green's theorem. See Goodman Chapter 3.5 for derivation



$$U(P_0)=\frac{1}{i\lambda_0}\iint_{\Sigma_1} U(P_1)\left(1-\frac{1}{ik_0 r_{01}}\right)\frac{\exp(ikr_{01})}{r_{01}}\frac{z}{r_{01}}ds_1$$

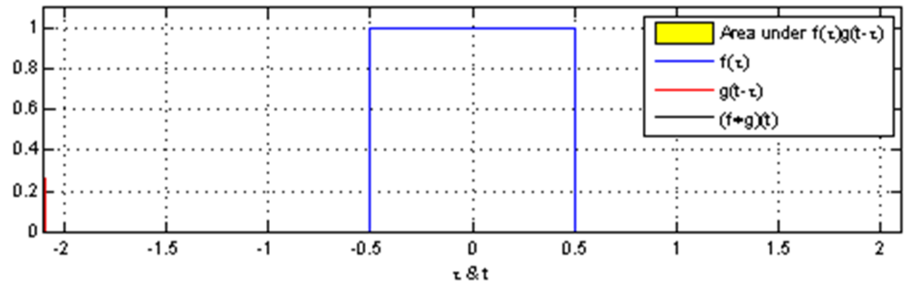
$$r_{01}=\sqrt{(x_0-x_1)^2+(y_0-y_1)^2+z^2}$$

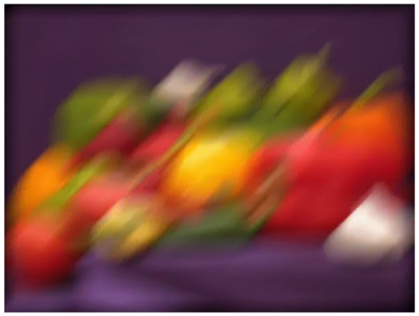
J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)

Reminder: Theorems of the FT

Convolution $$g(x,y) * h(x,y) = \iint_{-\infty}^{\infty} g(\xi,\eta) h(x-\xi, y-\eta) d\xi d\eta$$

$$\mathcal{F}\{g(x,y) * h(x,y)\} = G(f_x, f_y) H(f_x, f_y)$$

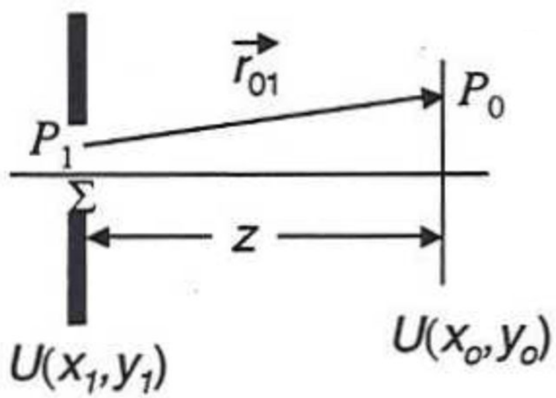




J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)
https://en.wikipedia.org/wiki/Convolution#/media/File:Convolution_of_box_signal_with_itself2.gif
Matlab "imfilter.m" documentation

Rayleigh-Sommerfeld solution

A solution can be obtained using Green's theorem. See Goodman Chapter 3.5 for derivation



$$U(P_0) = \frac{1}{i\lambda_0} \iint_{\Sigma_1} U(P_1) \left(1 - \frac{1}{ik_0 r_{01}}\right) \frac{\exp(ikr_{01})}{r_{01}} \frac{z}{r_{01}} ds_1$$

$$r_{01} = \sqrt{(x_0 - x_1)^2 + (y_0 - y_1)^2 + z^2}$$

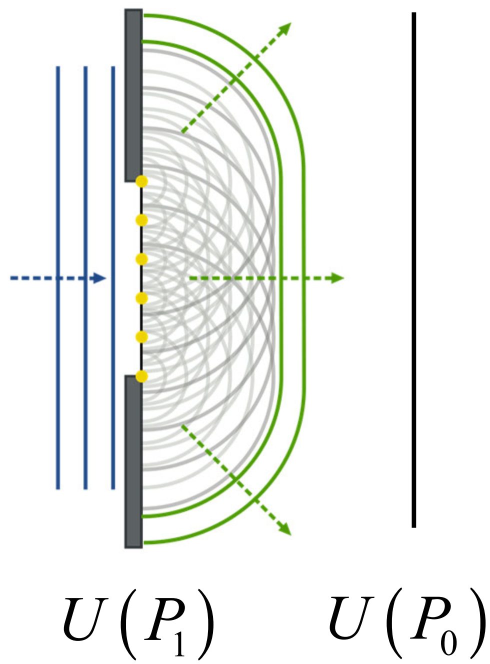
$$U(P_0) = U(P_1) * h(x_1, y_1)$$

$$h(x,y) = \frac{1}{i\lambda_0} \left(1 - \frac{1}{ik_0 r}\right) \frac{\exp(ikr)}{r} \frac{z}{r}$$

J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)

Rayleigh-Sommerfeld solution

A solution can be obtained using Green's theorem. See Goodman Chapter 3.5 for derivation



$$U(P_0) = U(P_1) * h(x_1, y_1)$$

$$h(x,y) = \frac{1}{i\lambda_0}\left(1 - \frac{1}{ik_0 r}\right)\frac{\exp(ikr)}{r}\frac{z}{r}$$

$$h(x,y) = \frac{\cos\theta}{i\lambda_0}\left(\frac{\exp(ikr)}{r} - \frac{\exp(ikr)}{ik_0 r^2}\right)$$

J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)
https://en.wikipedia.org/wiki/Huygens%E2%80%93Fresnel_principle

"Fun" fact

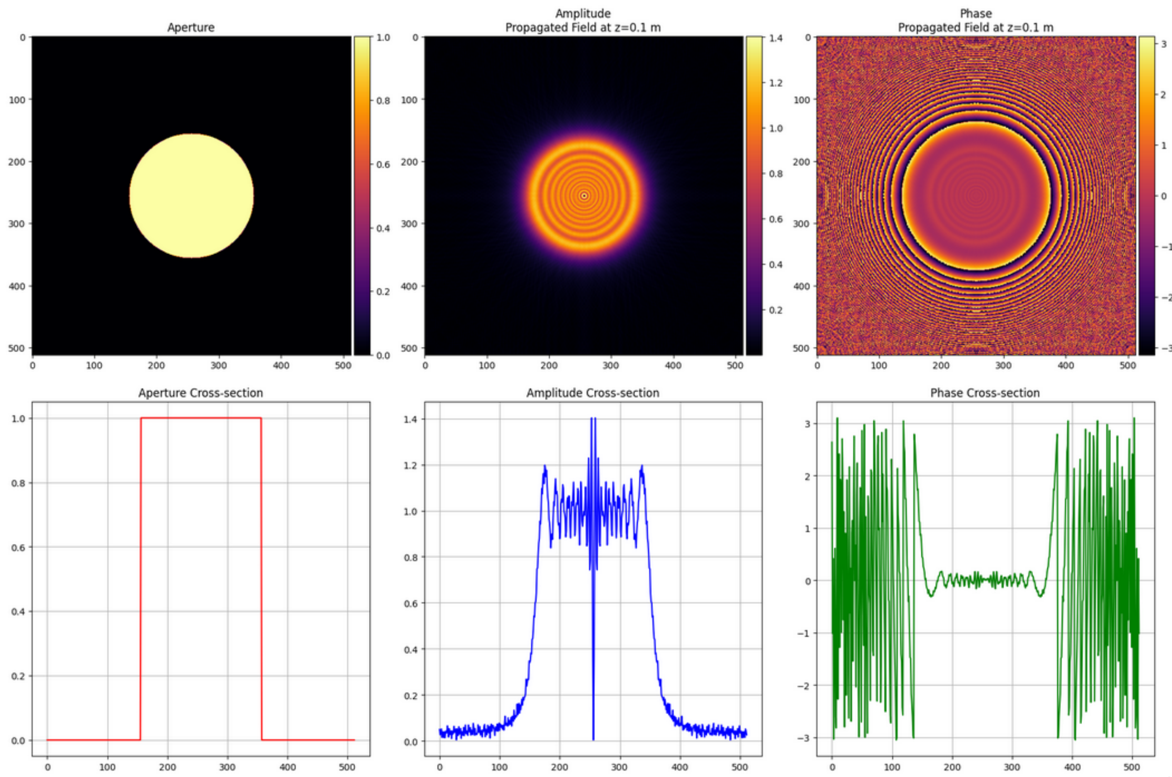
$$\mathcal{F}\left\{\frac{1}{i\lambda_0}\left(1-\frac{1}{ik_0 r}\right)\frac{\exp(ikr)}{r}\frac{z}{r}\right\}=\exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2-f_x^2-f_y^2}\right]$$

$$U(P_0)=U(P_1)*h(x_1,y_1) \quad \Longleftrightarrow \quad \mathcal{F}\{U(x,y,z)\}=\mathcal{F}\{U(x,y,0)\}H(f_x,f_y)$$

Both Rayleigh-Sommerfeld and angular spectrum are exact solutions of the Helmholz equation

Examples of propagation of different apertures

Angular_Spectrum_propagation.ipynb

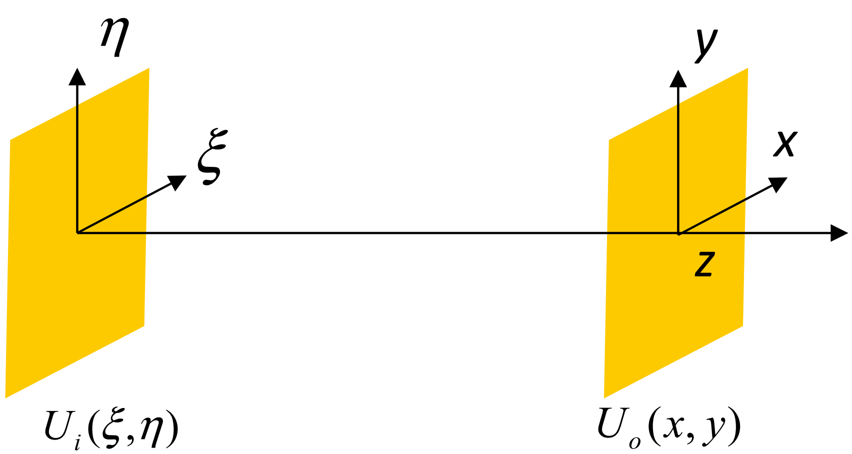


Fresnel approximation

will be useful, trust me

Fresnel approximation – paraxial or small angle

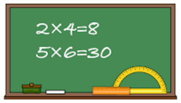
We take the Rayleigh-Sommerfeld solution



$$U_o(x,y) = \frac{1}{i\lambda_0} \iint U_i(\xi,\eta) \left(1 - \frac{1}{ik_0 r_{01}}\right) \frac{\exp(ikr_{01})}{r_{01}} \frac{z}{r_{01}} d\xi d\eta$$

$$r_{01} = \sqrt{z^2 + (x-\xi)^2 + (y-\eta)^2}$$

$$\frac{(x-\xi)^2 + (y-\eta)^2}{z^2} << 1$$



Read page 79 of J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)

Fresnel approximation

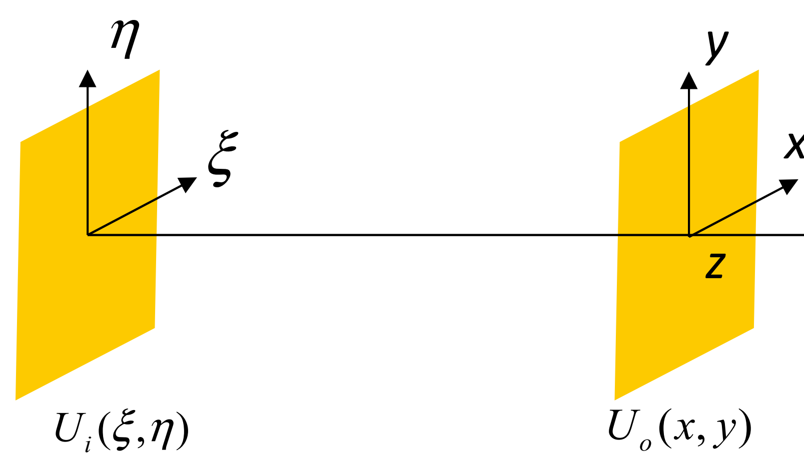
$$U_o(x,y)=\frac{\exp(ik_0z)}{i\lambda_0 z}\iint U_i(\xi,\eta)\exp\left(\frac{ik}{2z}\left[(x-\xi)^2+(y-\eta)^2\right]\right)d\xi d\eta$$

Convolution form

$$U_o(x,y)=U_i(x,y)*h(x,y)$$

$$h(x,y)=\frac{\exp(ik_0z)}{i\lambda_0 z}\exp\left(\frac{ik_0}{2z}\left[x^2+y^2\right]\right)$$

In this approximation each point makes a parabolic wavefront



Fresnel approximation

$$U_o(x,y)=\frac{\exp(ik_0z)}{i\lambda_0 z}\iint U_i(\xi,\eta)\exp\left(\frac{ik}{2z}\left[(x-\xi)^2+(y-\eta)^2\right]\right)d\xi d\eta$$

Convolution form

$$U_o(x,y)=U_i(x,y)*h(x,y)$$

$$h(x,y)=\frac{\exp(ik_0z)}{i\lambda_0 z}\exp\left(\frac{ik_0}{2z}\left[x^2+y^2\right]\right)$$

$$\tilde{U}_0(f_x,f_y)=\tilde{U}_i(f_x,f_y)H(f_x,f_y)$$

$$H(f_x,f_y)=\exp(ik_0z)\exp\left[-i\pi\lambda_0 z\left(f_x^{\,2}+f_y^{\,2}\right)\right]$$

Fresnel approximation

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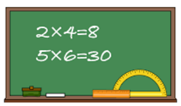
$$U_o(x,y)=\frac{\exp(ik_0z)}{i\lambda_0 z}\iint U_i(\xi,\eta)\exp\left(\frac{ik}{2z}\left[(x-\xi)^2+(y-\eta)^2\right]\right)d\xi d\eta$$



Fourier transform form

$$U_o(x,y)=\frac{\exp(ik_0z)}{i\lambda_0 z}\exp\left[\frac{ik_0}{2z}(x^2+y^2)\right]\iint U_i(\xi,\eta)\exp\left[\frac{ik_0}{2z}(\xi^2+\eta^2)\right]\exp\left(\frac{-i2\pi}{\lambda_0 z}(x\xi+y\eta)\right)d\xi d\eta$$

$$G(f_x,f_y)=\mathcal{F}\{g(x,y)\}=\iint_{-\infty}^{\infty} g(x,y)e^{-i2\pi(f_x x+f_y y)}dxdy$$

Fresnel approximation

Fourier transform form

$$U_o(x,y)=\frac{\exp(ik_0z)}{i\lambda_0 z}\exp\left[\frac{ik_0}{2z}(x^2+y^2)\right]\iint U_i(\xi,\eta)\exp\left[\frac{ik_0}{2z}(\xi^2+\eta^2)\right]\exp\left(\frac{-i2\pi}{\lambda_0 z}(x\xi+y\eta)\right)d\xi d\eta$$

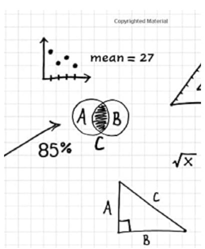
$$U_o(x,y)=\frac{\exp(ik_0z)}{i\lambda_0 z}\exp\left[\frac{ik_0}{2z}(x^2+y^2)\right]\mathcal{F}\left\{U_i(\xi,\eta)\exp\left[\frac{ik_0}{2z}(\xi^2+\eta^2)\right]\right\}_{f_x=\frac{x}{\lambda_0 z},\ f_y=\frac{y}{\lambda_0 z}}$$

$$G(f_x,f_y)=\mathcal{F}\{g(x,y)\}=\iint_{-\infty}^{\infty} g(x,y)e^{-i2\pi(f_x x+f_y y)}dxdy$$

“Fun” fact

Prove that the paraxial propagation transfer function is approximately equal to the angular spectrum transfer function for small angles

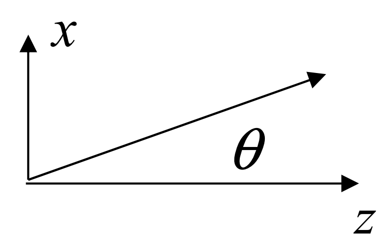
$$H\left(f_x, f_y\right) = \exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2 - f_x^2 - f_y^2}\right] \approx \exp\left(ik_0 z\right)\exp\left[-i\pi\lambda_0 z\left(f_x^{\,2} + f_y^{\,2}\right)\right]$$



When is the Fresnel approximation valid?

For small angles of propagation

$$2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2 - f_x^2 - f_y^2} \approx \exp\left(ik_0 z\right)\exp\left[-i\pi\lambda_0 z\left(f_x^2 + f_y^2\right)\right]$$



$$\lambda_0 f_x = \frac{\lambda_0}{2\pi}\left(2\pi f_x\right) = \frac{k_x}{k_0} = \sin\theta$$

$$\frac{z\sin^4\theta}{4\lambda_0} \ll 1$$

Example:

$\lambda_0 = 0.1\ \text{nm}$

$z = 1\ \text{m}$

$\theta \ll 0.0045\ \text{rad}$

Rule of thumb is actually much more relaxed +/- 5 degrees

When do we use the convolution vs FT forms?

There are tricks we can play to use these different forms and minimize sampling and computational requirements

Depending on your problem, you can use one or a combination of these propagators

Dr. Abraham Levitan
Computational X-ray Imaging, PSI
Numerical propagation

$$H\left(f_x, f_y\right) = \exp\left(ik_0 z\right)\exp\left[-i\pi\lambda_0 z\left(f_x^{\,2} + f_y^{\,2}\right)\right]$$

$$U_0\left(x, y\right) = \mathcal{F}^{-1}\left\{\mathcal{F}\left\{U_i\left(x, y\right)\right\} H\left(f_x, f_y\right)\right\}$$

$$U_o\left(x, y\right) = \frac{\exp\left(ik_0 z\right)}{i\lambda_0 z}\exp\left[\frac{ik_0}{2z}\left(x^2 + y^2\right)\right]\mathcal{F}\left\{U_i\left(\xi, \eta\right)\exp\left[\frac{ik_0}{2z}\left(\xi^2 + \eta^2\right)\right]\right\}_{f_x = \frac{x}{\lambda_0 z},\; f_y = \frac{y}{\lambda_0 z}}$$

Fraunhofer approximation – the far field

Fraunhofer approximation

Fresnel approximation in Fourier transform form

$$U_o(x,y)=\frac{\exp(ik_0 z)}{i\lambda_0 z}\exp\left[\frac{ik_0}{2z}(x^2+y^2)\right]\iint U_i(\xi,\eta)\exp\left[\frac{ik_0}{2z}(\xi^2+\eta^2)\right]\exp\left(\frac{-i2\pi}{\lambda_0 z}(x\xi+y\eta)\right)d\xi d\eta$$

$$z\gg\frac{k_0}{2}(\xi^2+\eta^2)=\frac{\pi}{\lambda_0}(\xi^2+\eta^2)$$

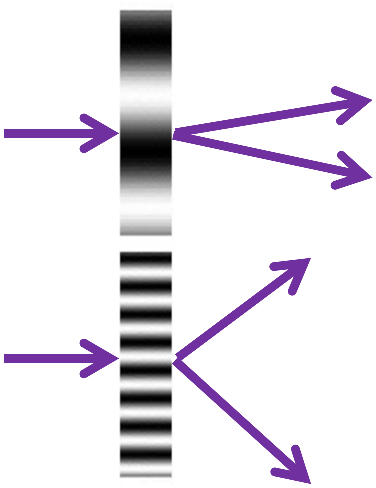
$$U_o(x,y)=\frac{\exp(ik_0 z)}{i\lambda_0 z}\exp\left[\frac{ik_0}{2z}(x^2+y^2)\right]\iint U_i(\xi,\eta)\exp\left(\frac{-i2\pi}{\lambda_0 z}(x\xi+y\eta)\right)d\xi d\eta$$

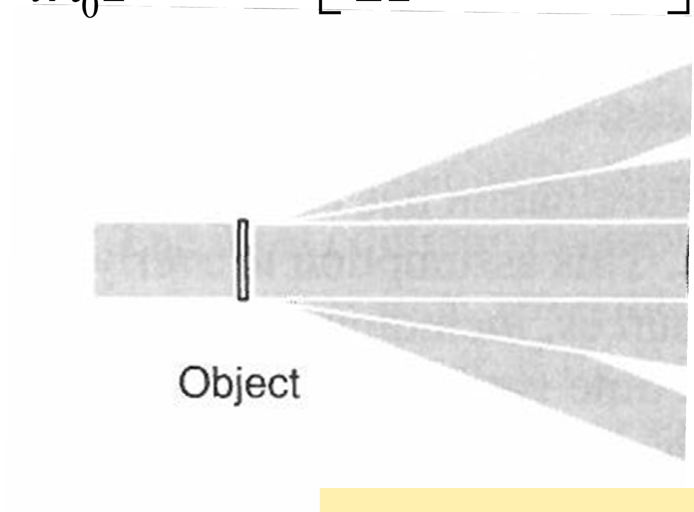
$$G(f_x,f_y)=\mathcal{F}\{g(x,y)\}=\iint_{-\infty}^{\infty} g(x,y)e^{-i2\pi(f_x x+f_y y)}dxdy$$

Fraunhofer approximation

Propagation far enough basically computes a Fourier transform

$$U_o(x,y) = \frac{\exp(ik_0 z)}{i\lambda_0 z} \exp\left[\frac{ik_0}{2z}\left(x^2+y^2\right)\right] \mathcal{F}\left\{U_i(\xi,\eta)\right\}_{\substack{f_x=\frac{x}{\lambda_0 z} \\ f_y=\frac{y}{\lambda_0 z}}}$$





J. W. Goodman, Introduction to Fourier Optics, fourth edition. McMillan learning (2017)

$$G(f_x, f_y) = \mathcal{F}\{g(x,y)\} = \iint_{-\infty}^{\infty} g(x,y) e^{-i2\pi(f_x x + f_y y)} dx dy$$

Fraunhofer approximation

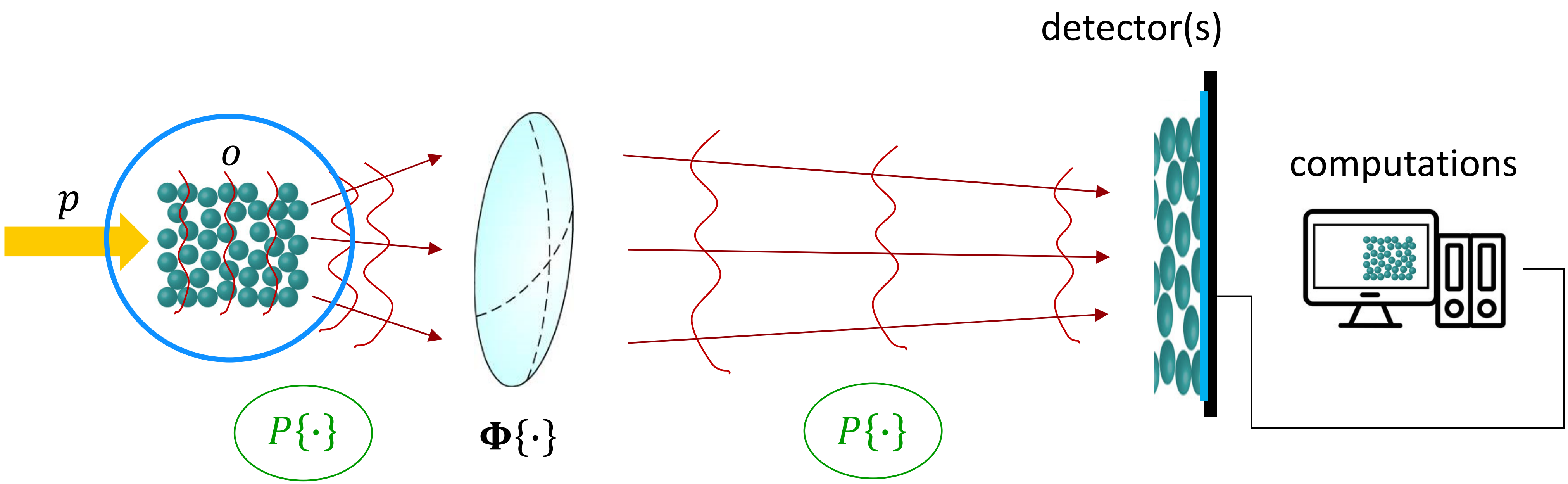
PSI
EPFL

$$z \gg \frac{\pi D^2}{\lambda_0}$$

Optical regime:	D = 2 cm, λ = 600 nm,	z >> 2.09 km
	D = 1 mm, λ = 600 nm,	z >> 5.23 m
X-ray regime:	D = 2 µm, λ = 0.2 nm,	z >> 6.28 cm

Free-space propagators done

A more detailed model



Interaction of beam with the sample

Paraxial wave equation and projection approximation

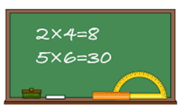
Back to Helmholtz equation

The sample interaction is given by the index of refraction being not constant in space

$$\left[\nabla^2 + k_0^{\,2} n^2(\mathbf{r})\right]\psi(\mathbf{r}) = 0$$

Ansatz of a field mostly propagating and changing in the z direction, the envelope will change slowly as a function of z

$$\psi(x,y,z) = \tilde{\psi}(x,y,z)\exp(ik_0 z)$$



$$\left\{2ik_0\frac{\partial}{\partial z} + \nabla_t^{\,2} + k_0^{\,2}\left[n^2(x,y,z) - 1\right]\right\}\tilde{\psi}(x,y,z) = 0$$

“Fun” fact

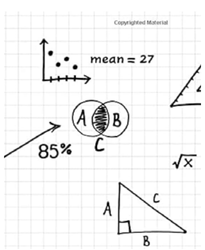
Prove that the Fresnel approximation satisfies the paraxial wave equation

$$U_o(x,y)=\frac{\exp(ik_0 z)}{i\lambda_0 z}\iint U_i(\xi,\eta)\exp\left(\frac{ik}{2z}\left[(x-\xi)^2+(y-\eta)^2\right]\right)d\xi d\eta$$

Hint: remember the equation below we already took into account the z exponential

$$U_0(x,y,z)=\tilde{\psi}(x,y,z)\exp(ik_0 z)$$

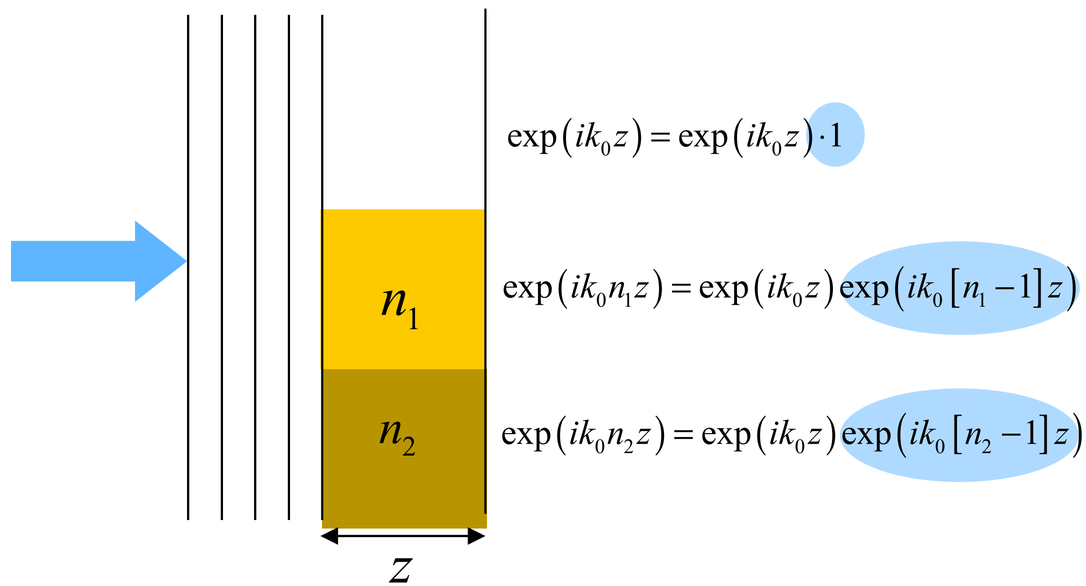
$$\left\{2ik_0\frac{\partial}{\partial z}+\nabla_t^{\,2}\right\}\tilde{\psi}(x,y,z)=0$$



Projection approximation

The object is thin enough, and boring enough, that we can ignore any diffraction within it

$$n = 1 - \delta + i\beta$$



Projection approximation

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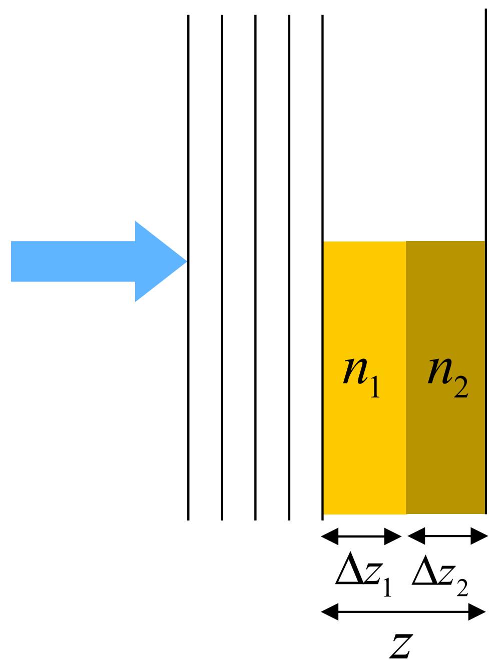


$$\exp(ik_0 z) = \exp(ik_0 z) \cdot 1$$

$$\exp(ik_0 n_1 \Delta z_1)\exp(ik_0 n_2 \Delta z_2) = \exp(ik_0 z)\exp(ik_0 [n_1 \Delta z_1 + n_2 \Delta z_2 - 1])$$

Projection approximation

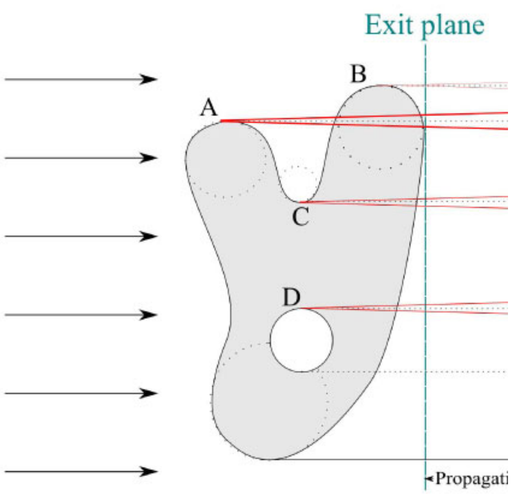
The object is thin enough, and boring enough, that we can ignore any diffraction within it

$$\tilde{\psi}(x,y,z=z_1) \approx \tilde{\psi}(x,y,z=z_0)\,o(x,y)$$

$$o(x,y) = \exp\left(ik_0 z\right)\exp\left\{ik_0\int_0^z [n(x,y,z)-1]dz\right\}$$

$n = 1 - \delta + i\beta$

Index of refraction is complex-valued



K. S. Morgan, K. K. W. Siu, and D. M. Paganin, "The projection approximation and edge contrast for x-ray propagation-based phase contrast imaging of a cylindrical edge," Opt. Express **18**, 9865 (2010).

Projection approximation

$$\tilde{\psi}(x,y,z=z_1) \approx \tilde{\psi}(x,y,z=z_0)\, o(x,y)$$

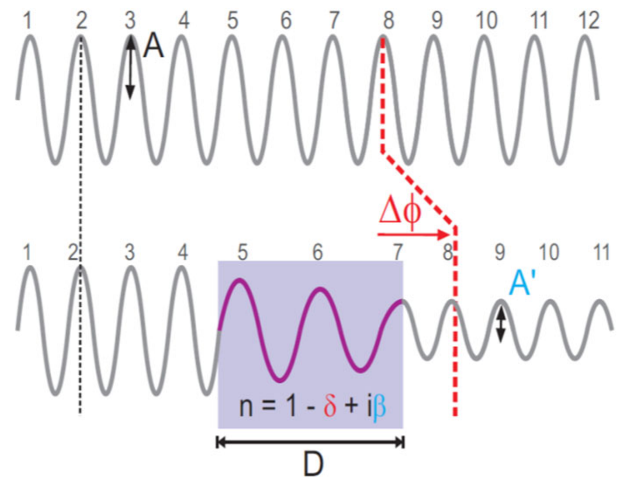
$$o(x,y) = \exp\left\{ik_0 \int_0^z [n(x,y,z)-1]dz\right\}$$

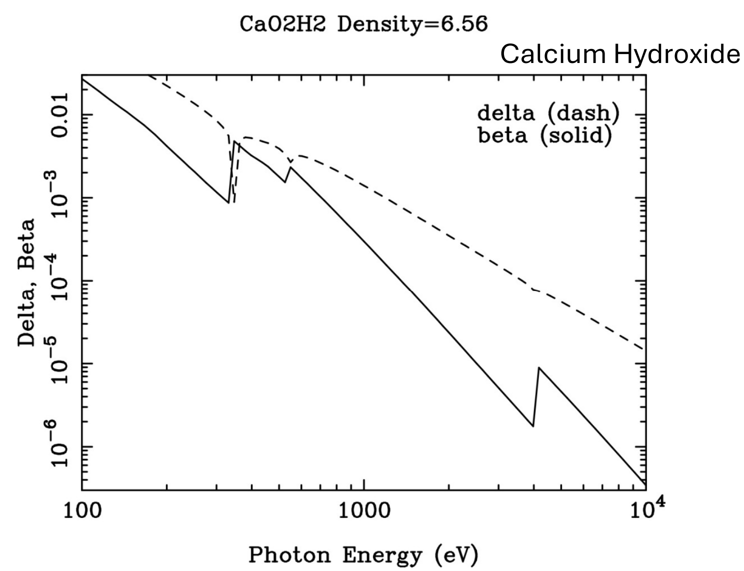
$$o(x,y) = A(x,y)\exp\left(i\phi(x,y)\right)$$

$$n = 1 - \delta + i\beta$$

$$A(x,y) = \exp\left(-k_0 \int_0^z \beta(x,y,z)dz\right)$$

$$\phi(x,y) = -k_0 \int_0^z \delta(x,y,z)dz$$





Images from C. Grünzweig, PhD thesis, ETH-Zürich (2009), CXRO

Multislice propagation

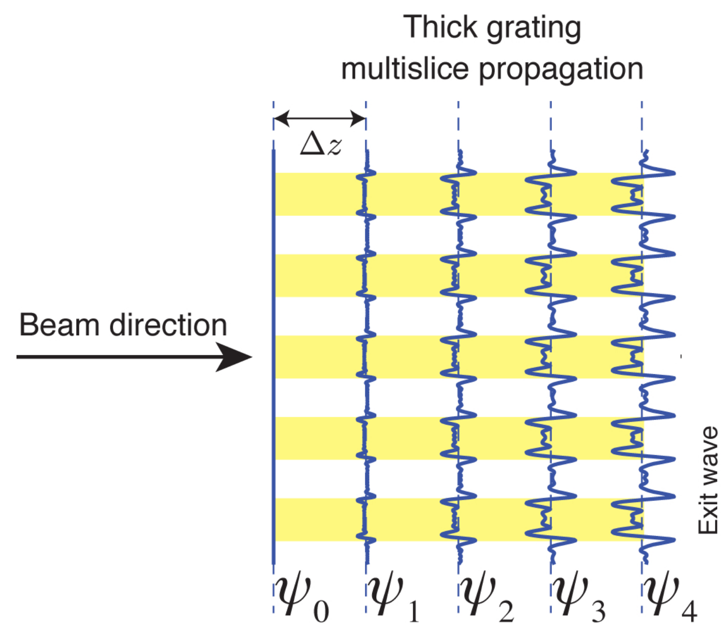
Pioneered for simulating elastic scattering of electrons (Cowley and Moodie)

$$o_n(x,y) = \exp\left\{ik_0 \int_{z_n}^{z_{n+1}} [n(x,y,z)-1]dz\right\}$$

Make very thin slices and sequentially apply the transmissivity followed by the propagation

$$\psi_{n+1}(x,y) = \mathcal{P}_{\Delta z}\{\psi_n(x,y)o_n(x,y)\}$$

$$\mathcal{P}_{\Delta z}\{\cdot\} = \mathcal{F}^{-1}\left\{\mathcal{F}\{\cdot\}\exp\left[i2\pi z\sqrt{\left(\frac{k_0}{2\pi}\right)^2 - f_x^2 - f_y^2}\right]\right\}$$



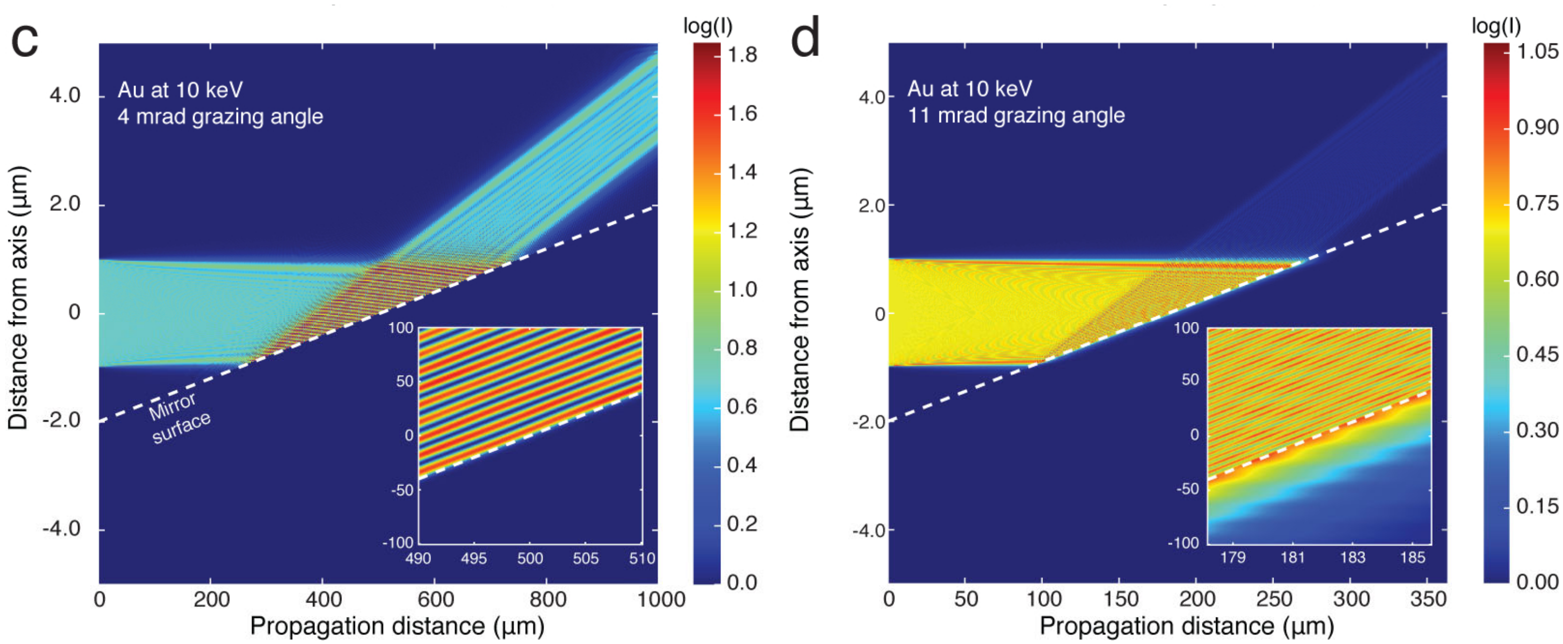
J. M. Cowley and A. F. Moodie, "The Scattering of Electrons by Atoms and Crystals. I. A New Theoretical Approach," Acta Cryst. **10** (1957)

K. Li, M. Wojcik, and C. Jacobsen, "Multislice does it all—calculating the performance of nanofocusing X-ray optics," Opt. Express **25**, 1831 (2017)

Multislice propagation

Calculation of reflection from an X-ray mirror showing

- Interference standing waves
- Total external reflection with evanescent wave



K. Li, M. Wojcik, and C. Jacobsen, "Multislice does it all—calculating the performance of nanofocusing X-ray optics," Opt. Express **25**, 1831 (2017)

Beer-lambert law

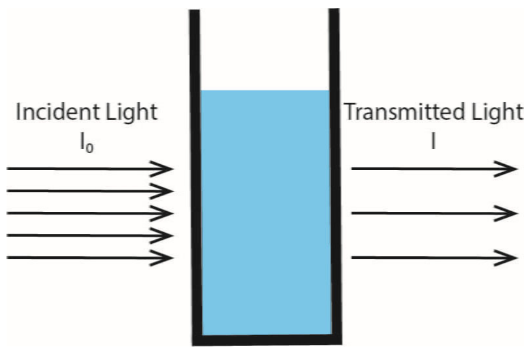
Beer-lambert law

Popular principle quoted in X-ray tomography
“Lambert expressed the law, which states that the loss of light intensity when it propagates in a medium is directly proportional to intensity and path length, in the mathematical form used today”

$$\Delta I = -\mu I \Delta z$$

$$\frac{\partial I}{\partial z} = -\mu I$$

$$I = I_0 \exp(-\mu z)$$



$$I(x,y) = I_0(x,y)\exp\left(-\int \mu(x,y,z)dz\right)$$


Johann Heinrich Lambert (1728–1777)


August Beer (1825–1863)

https://en.wikipedia.org/wiki/Beer%E2%80%93Lambert_law

Beer-lambert law

$$I(x,y) = I_0(x,y)\exp\left(-\int_{z_0}^{z_1}\mu(x,y)dz\right)$$

$$\tilde{\psi}(x,y,z=z_1) \approx \tilde{\psi}_0(x,y,z=z_0)\,o(x,y)$$

$$o(x,y) = \exp\left(-k_0\int_{z_0}^{z_1}\beta(x,y,z)dz\right)\exp\left(-ik_0\int_{z_0}^{z_1}\delta(x,y,z)dz\right)$$

$$\left|\tilde{\psi}(x,y,z=z_1)\right|^2 \approx \left|\tilde{\psi}_0(x,y,z=z_0)\right|^2 \exp\left(-2k_0\int_{z_0}^{z_1}\beta(x,y,z)dz\right)$$

$$\mu(x,y,z) = -2k_0\beta(x,y,z)$$

Absorption coefficient

$$L = \frac{1}{\mu}$$

Attenuation length

https://en.wikipedia.org/wiki/Beer%E2%80%93Lambert_law

Free-space propagators and interaction with sample done

A more detailed model