1.1 Introduction, Fourier, Fraunhofer, Compton, and Thomson

Scattering
Block Course
12.-13.02.2024

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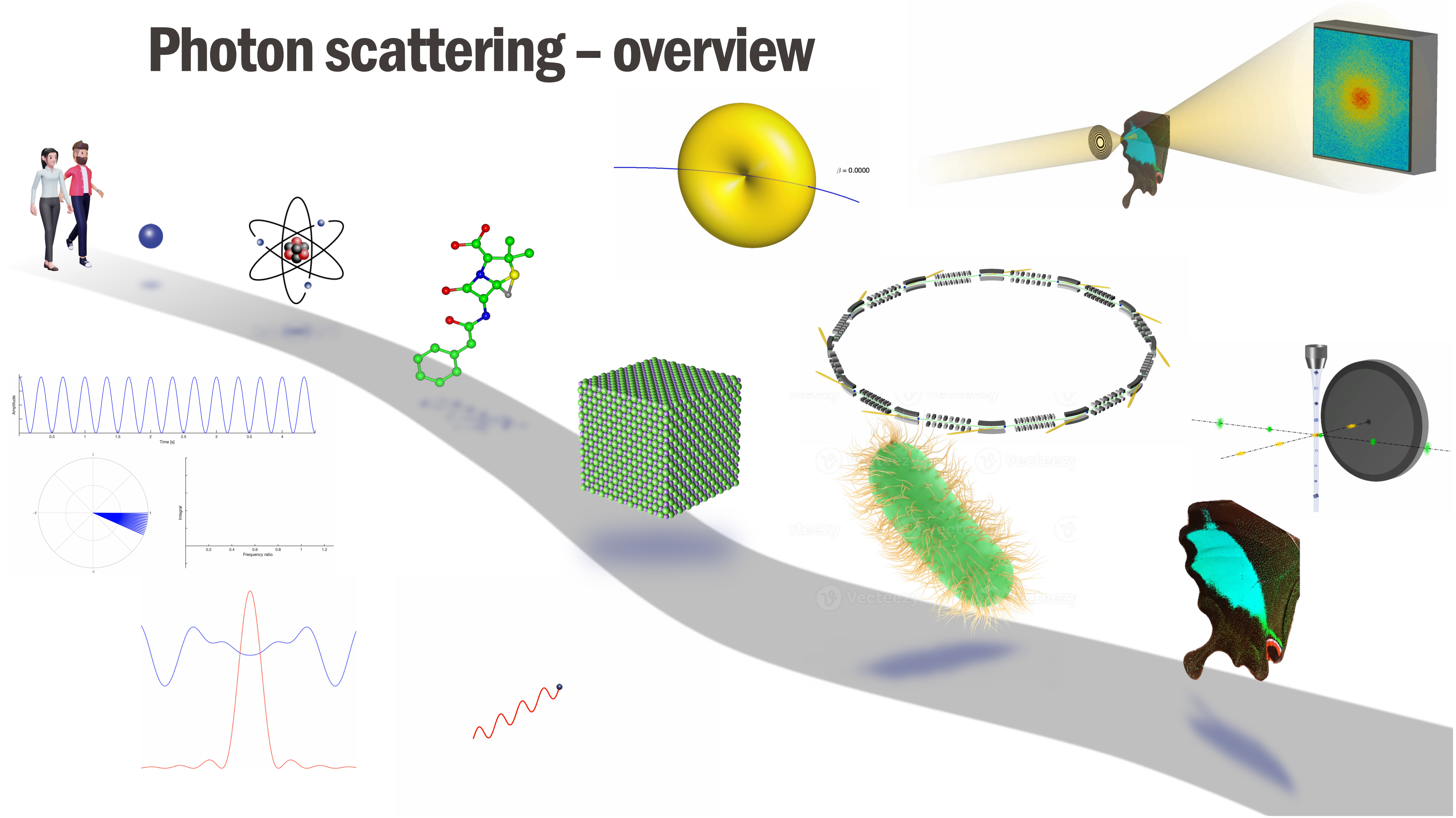
University of Zurich[UZH]

Photon scattering – overview



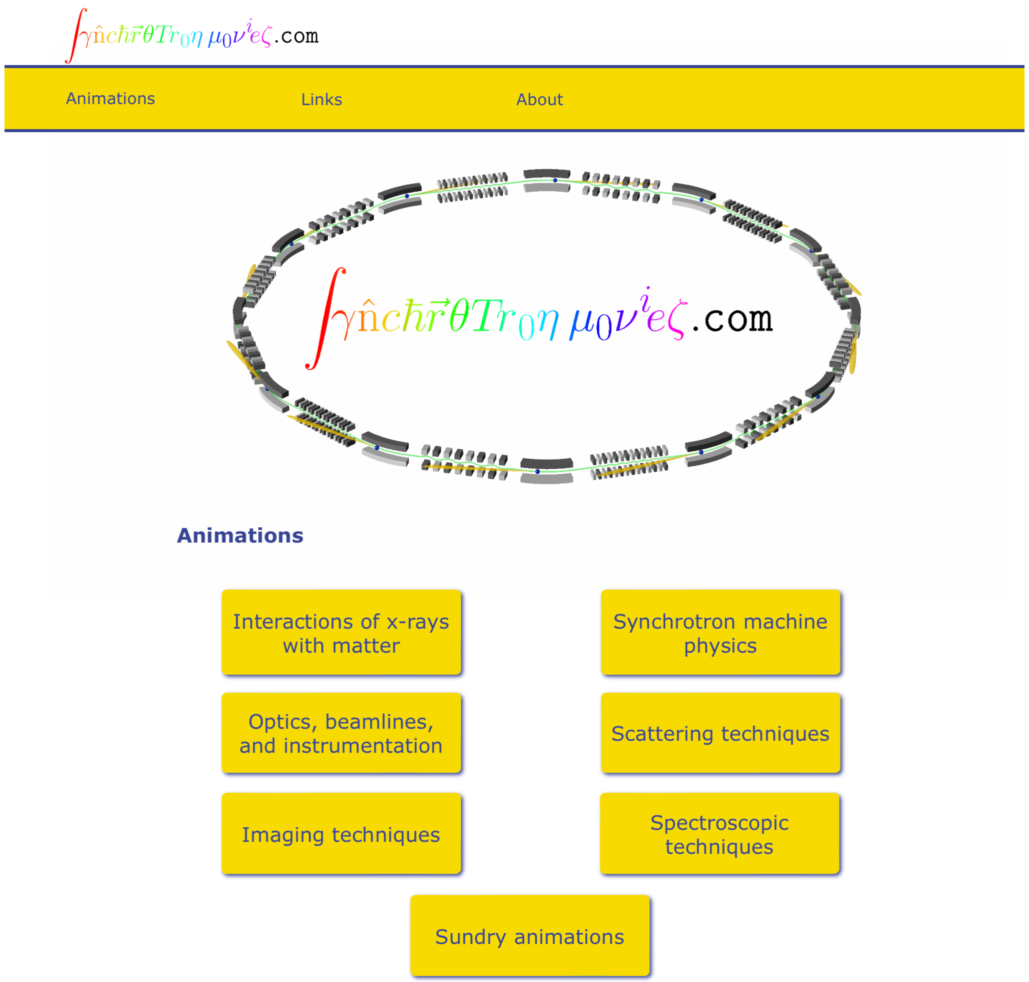
Photon scattering – overview

- Today
  - FTs – how they work
  - Far-field scattering pattern = FT
  - Electric and magnetic forces
  - Dipole radiation
  - Compton and Thomson scattering

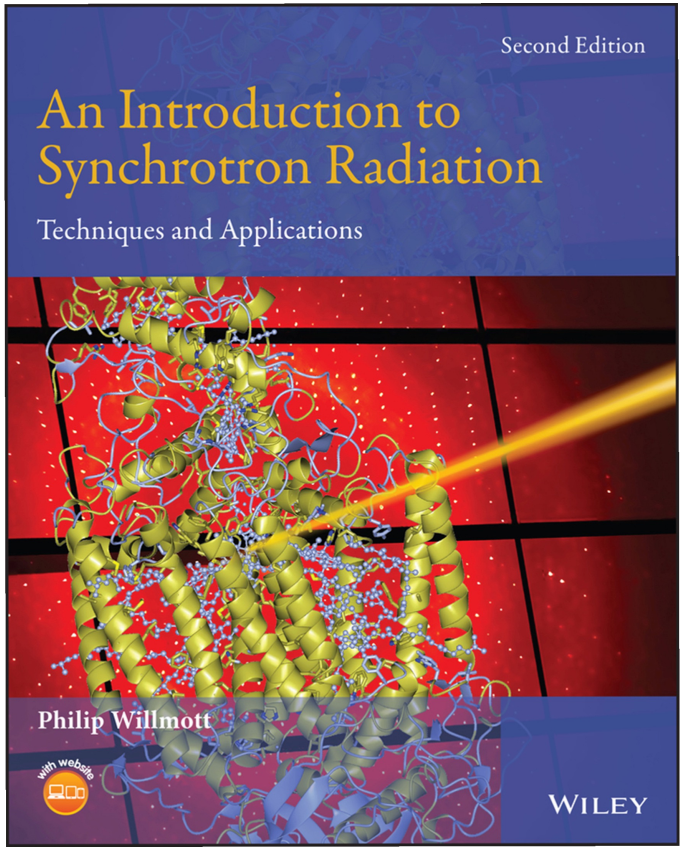
  - Relativistic dipole radiation
  - Atomic form factors
  - Structure factors
  - The complex refractive index
  - Anomalous diffraction
- Tomorrow
  - Single-crystal diffraction
    - Laue
    - Monochromatic
  - Powder diffraction
  - Surface diffraction

  - Small-angle x-ray scattering
  - X-ray reflectometry
  - Speckle
  - Coherent x-ray diffractive imaging
  - Ptychography

Useful material and links

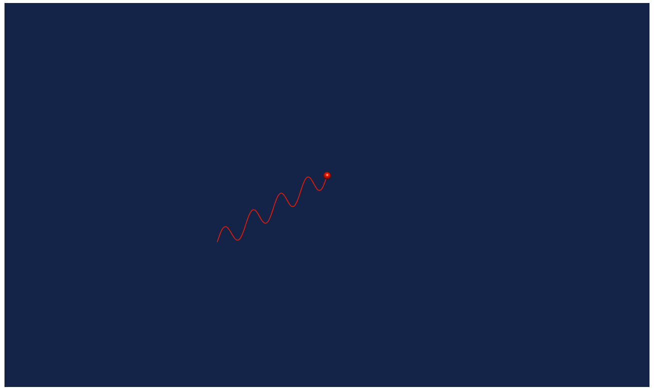


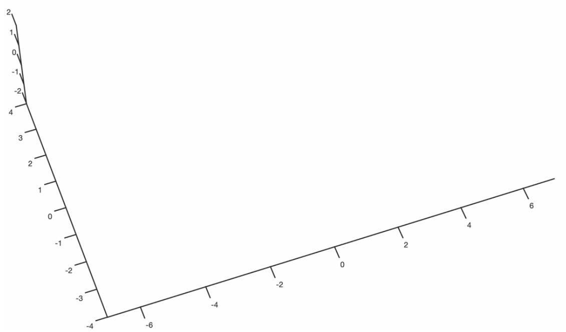
https://www.synchrotronmovies.com

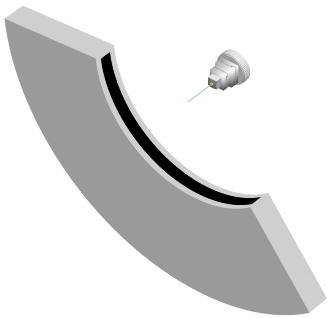


https://www.wiley.com/en-us/An+Introduction+to+Synchrotron+Radiation%3A+Techniques+and+Applications%2C+2nd+Edition-p-9781119280392

Useful material and links







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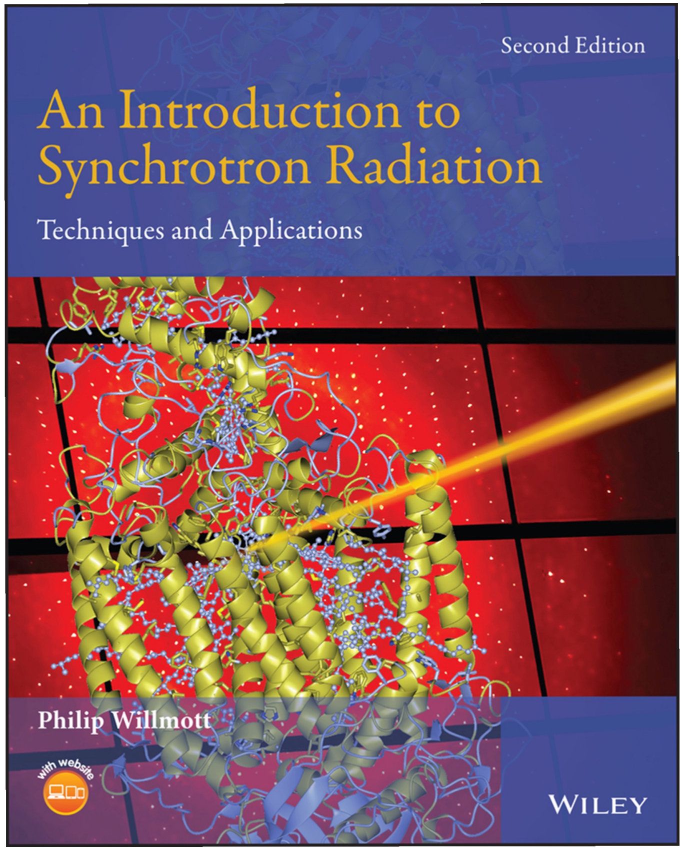
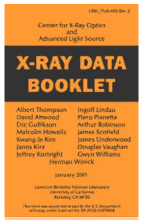


https://www.wiley.com/en-us/An+Introduction+to+Synchrotron+Radiation%3A+Techniques+and+Applications%2C+2nd+Edition-p-9781119280392

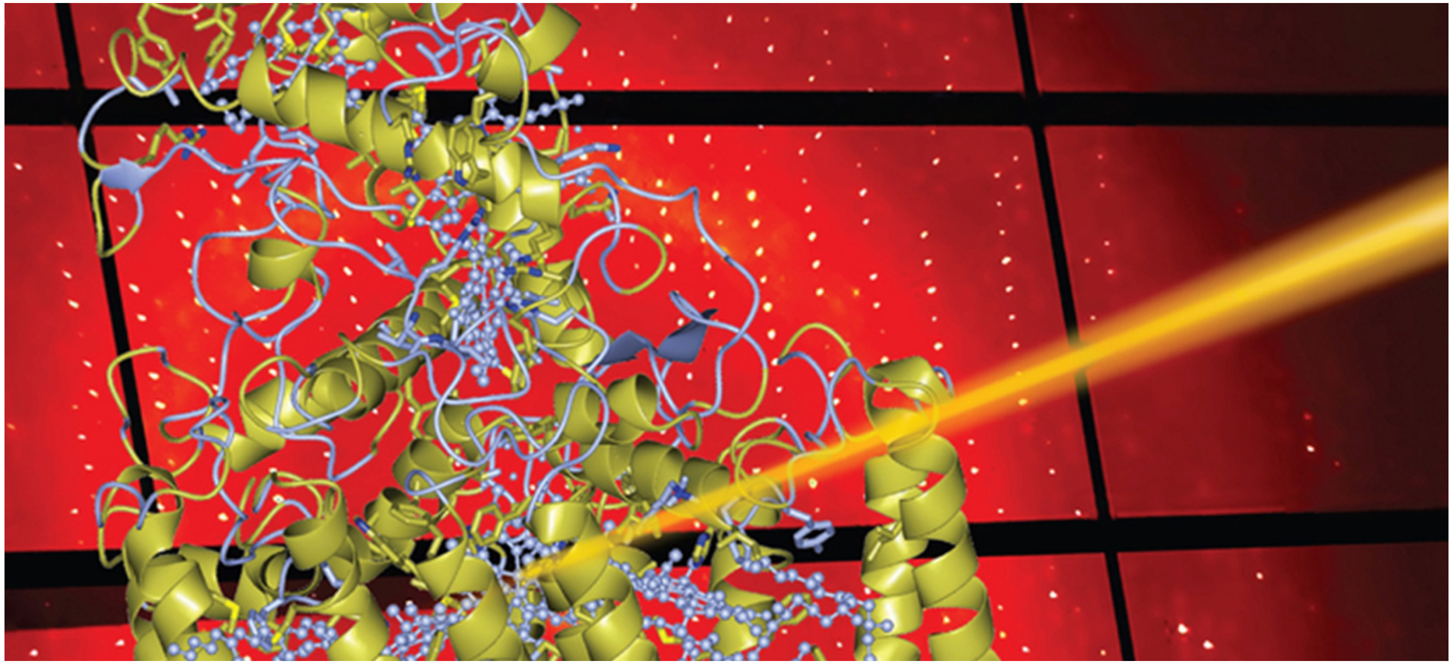
Other online resources

- 400+ figures from book
  - https://wiley.mpstechnologies.com/wiley/BOBContent/searchLPBobContent.do
    Type “Willmott” into author field
- Center for x-ray optics CXRO: http://www.cxro.lbl.gov/
  - Interactions of x-rays with matter – plots, databases, x-ray data booklet
  - Educational material on x-ray optics, nanofabrication, coatings, etc.



- X-ray cross-section database
  - https://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html
- Atomic form factors
  - http://lampx.tugraz.at/~hadley/ss1/crystaldiffraction/atomicformfactors/formfactors.php
- Protein data bank
  - https://www.rcsb.org/
- XAS data base
  - http://cars.uchicago.edu/xaslib/search
- EXAFS spectra
  - http://www.exafsmaterials.com/Ref_Spectra_0.4MB.pdf
- Anomalous structure factor calculator
  - http://cars9.uchicago.edu/dafs/diffkk/
- Darwin-width calculator
  - https://www.chess.cornell.edu/users/calculators/x-ray-calculations-darwin-width
- X-ray optics intro
  - http://www.x-ray-optics.de/index.php/en/

Massive open online courses (MOOCs)



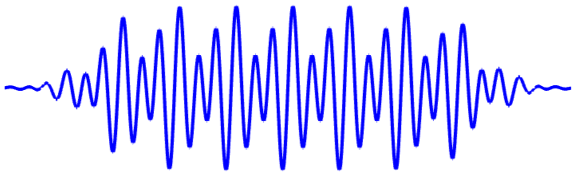
EPFL: 2 six-week courses

- Introduction to synchrotron and XFEL radiation – Part 1
- Introduction to synchrotron and XFEL radiation – Part 2

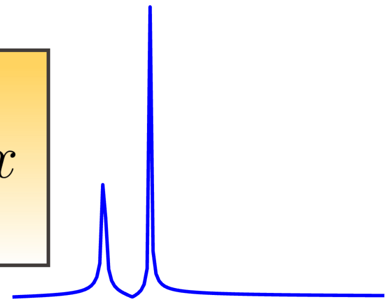
Fourier transforms and far-field scattering

How does a Fourier transform work?

$g(x)$



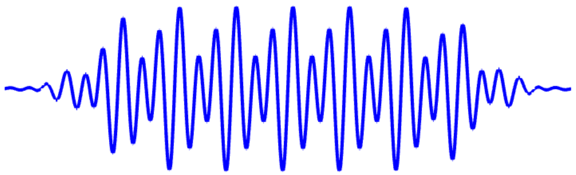
$$\mathcal{F}\{g(x)\} = \int_a^b g(x)\, e^{-ikx}\, dx$$



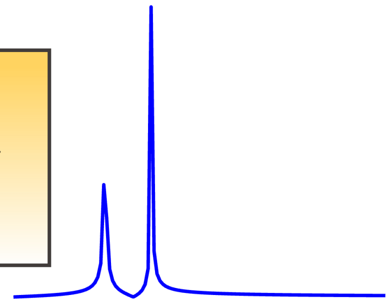
$$k = 2\pi/\lambda = 2\pi f/c$$

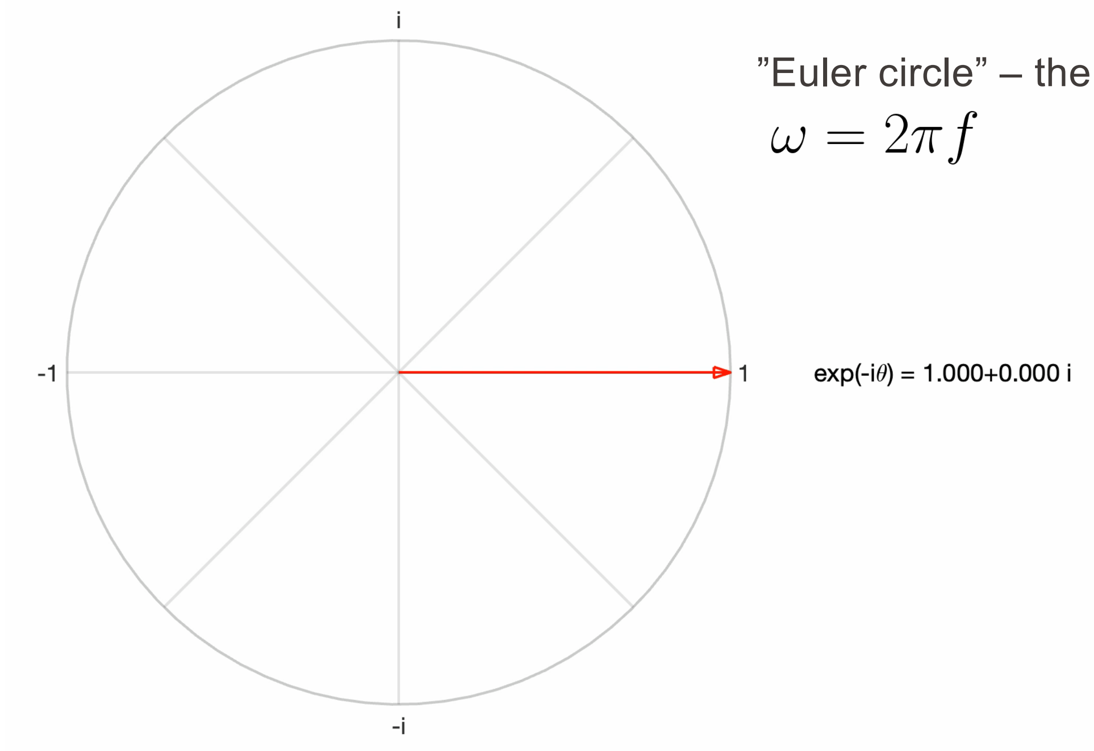
Drawn heavily from: https://www.youtube.com/watch?v=spUNpyF58BY&list=WL&index=72

How does a Fourier transform work?

$g(t)$ 

$$\mathcal{F}\{g(t)\} = \int_a^b g(t)\,e^{-i\omega t}\,dt$$





"Euler circle" – the engine of an FT

$$\omega = 2\pi f$$

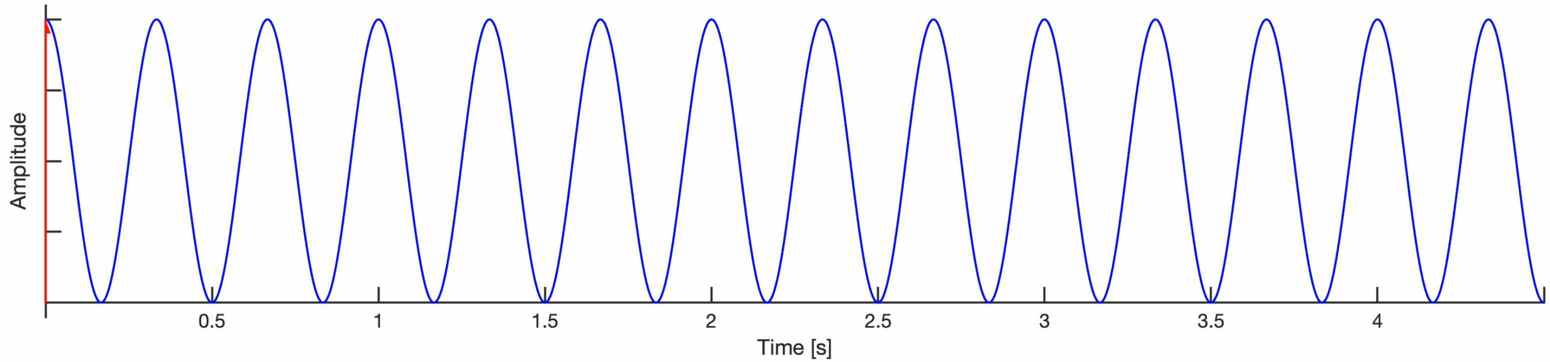
Euler's equation

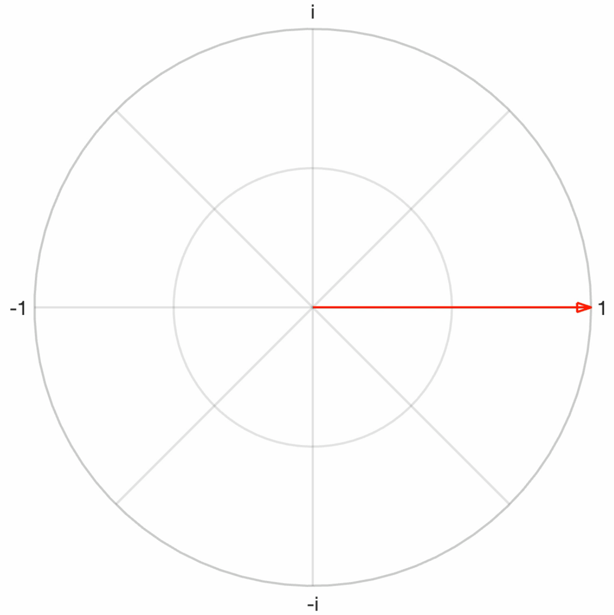
$$e^{i\theta} = \cos\theta + i\sin\theta$$

https://www.youtube.com/watch?v=4hxpA-SPiRQ&t=11s

How does a Fourier transform work?

$g(t)$



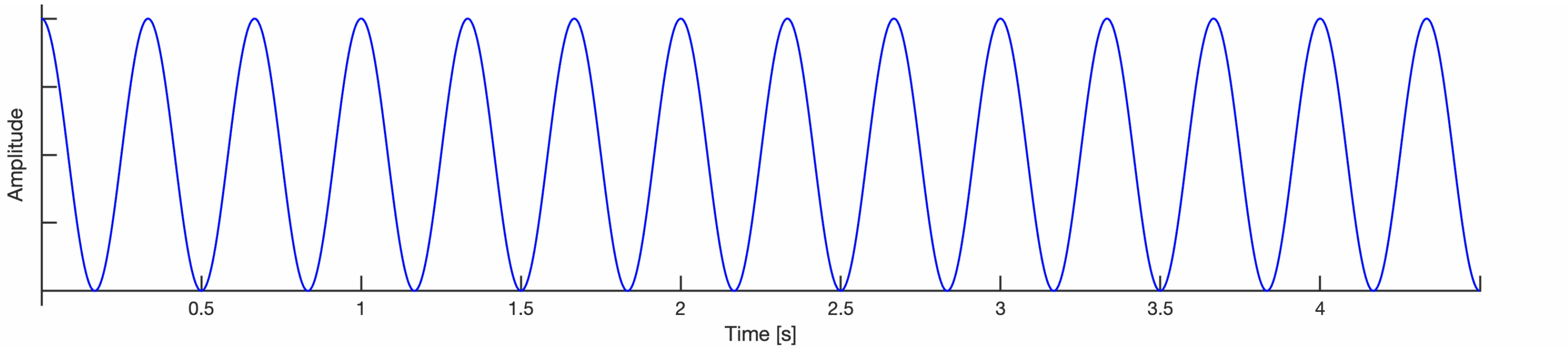


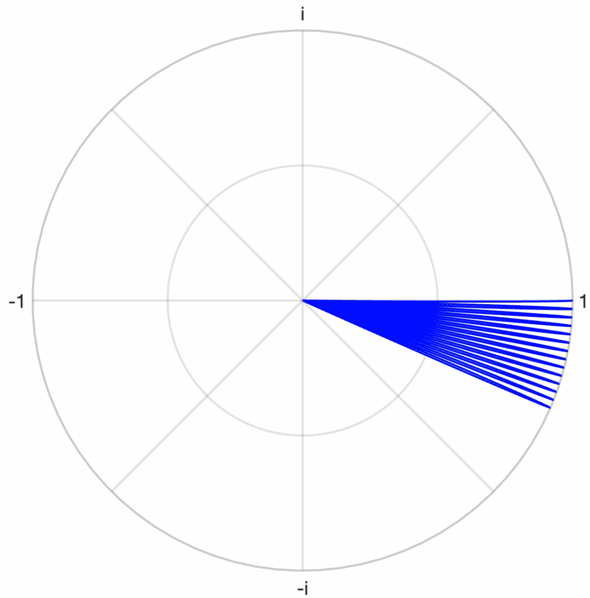
$g(t)\, e^{-i\omega t}$

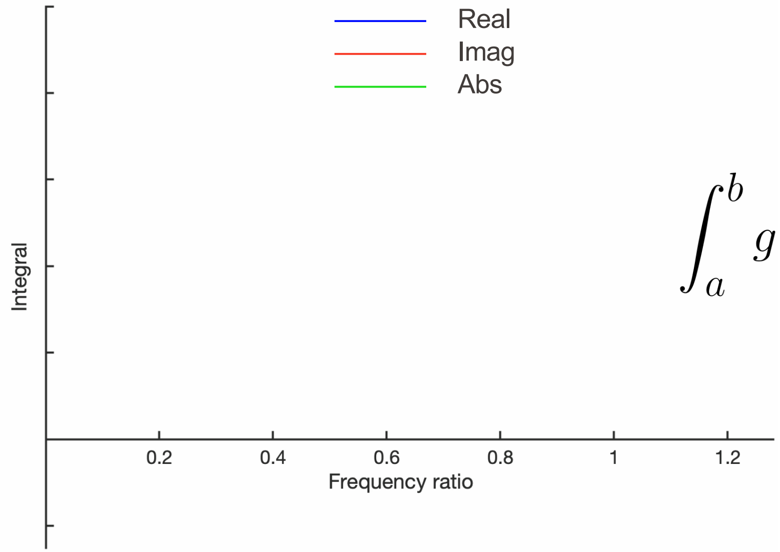
N.B. Two different frequencies

- $g(t)$: $f = \omega_{g(t)}/2\pi = 3\,\mathrm{Hz}$
- Euler circle: $f = \omega/2\pi$

How does a Fourier transform work?



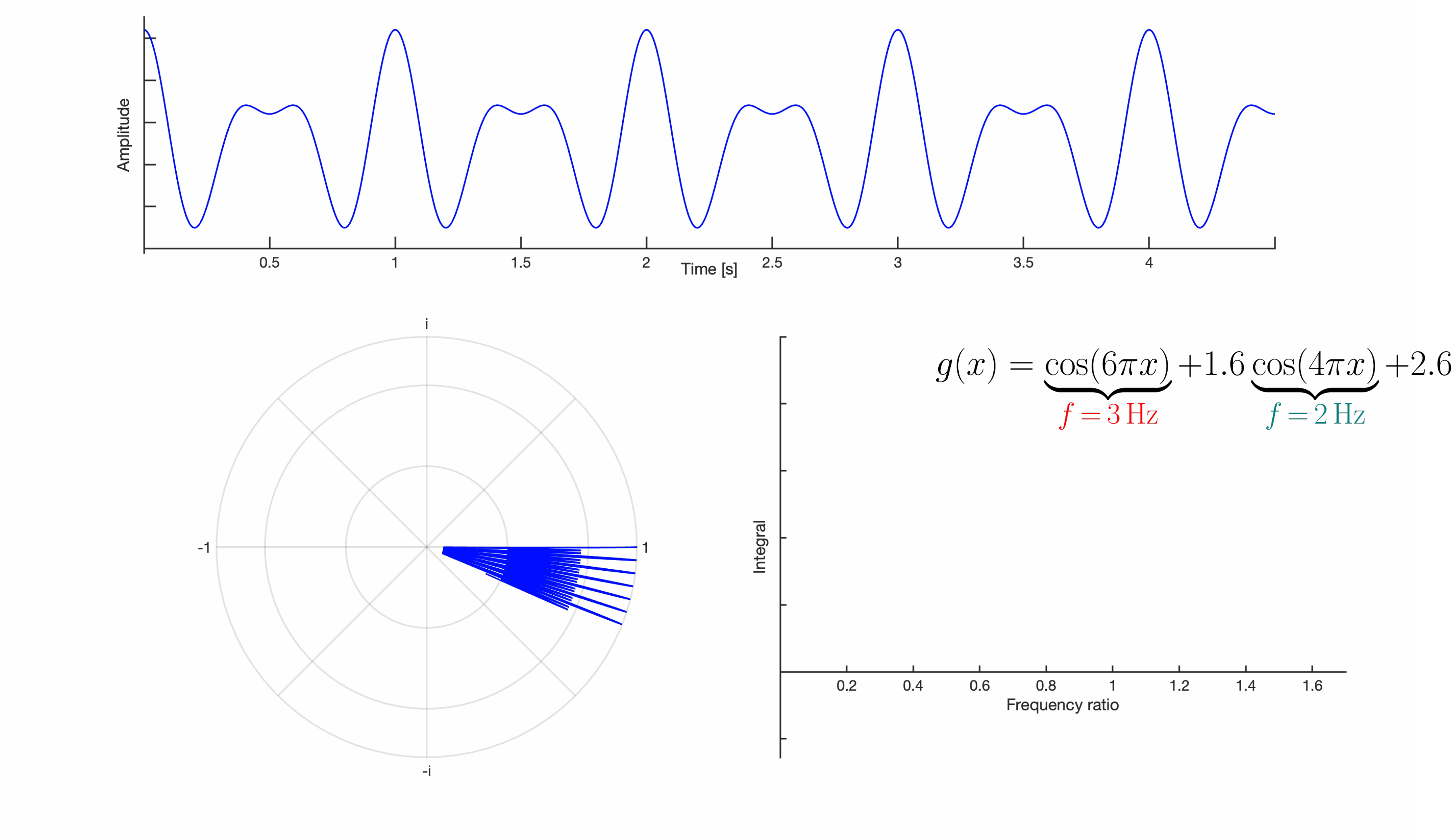




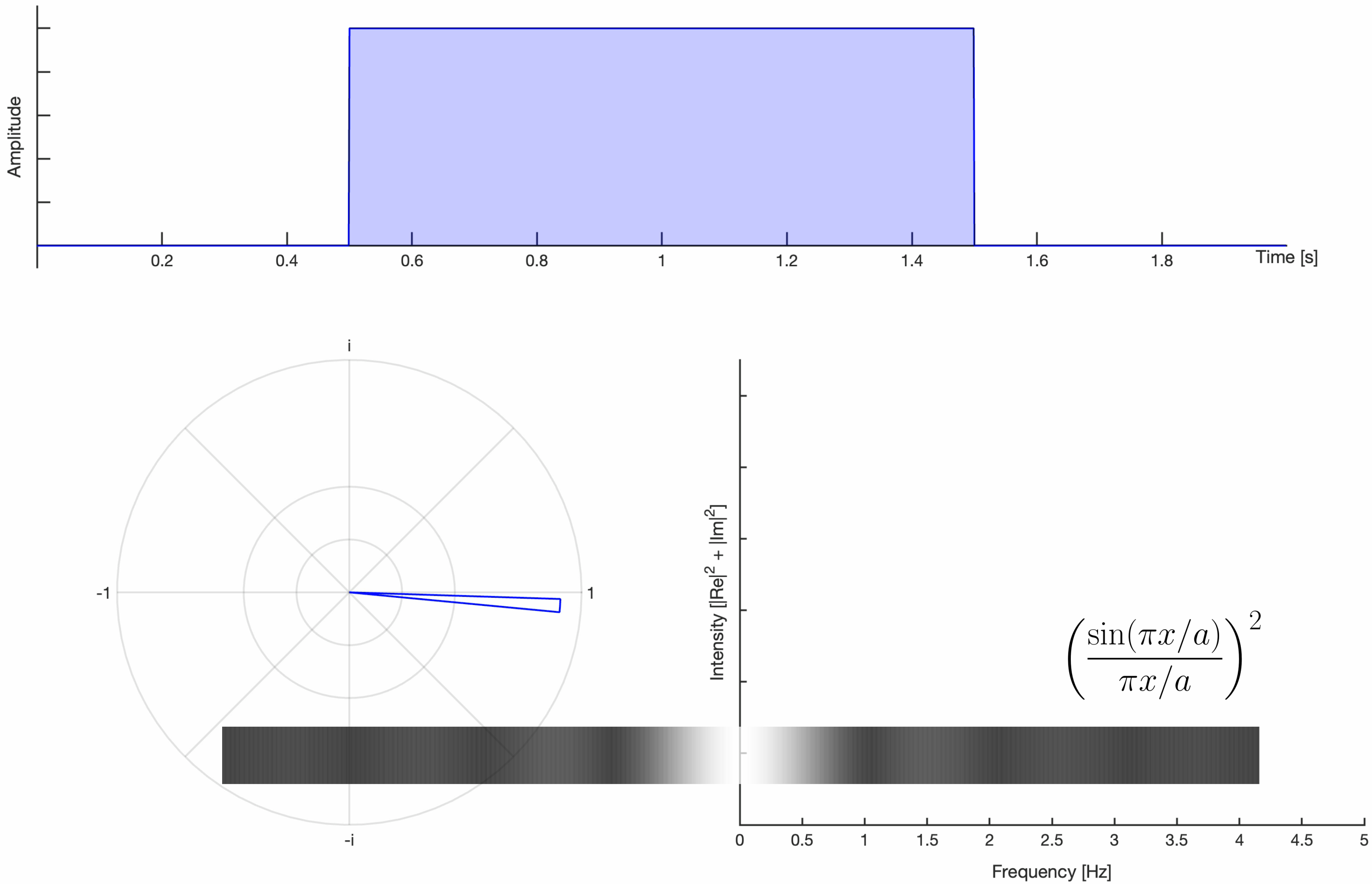
Vary this

$$\int_a^b g(t)\, e^{-i\omega t}\, dt$$

How does a Fourier transform work?

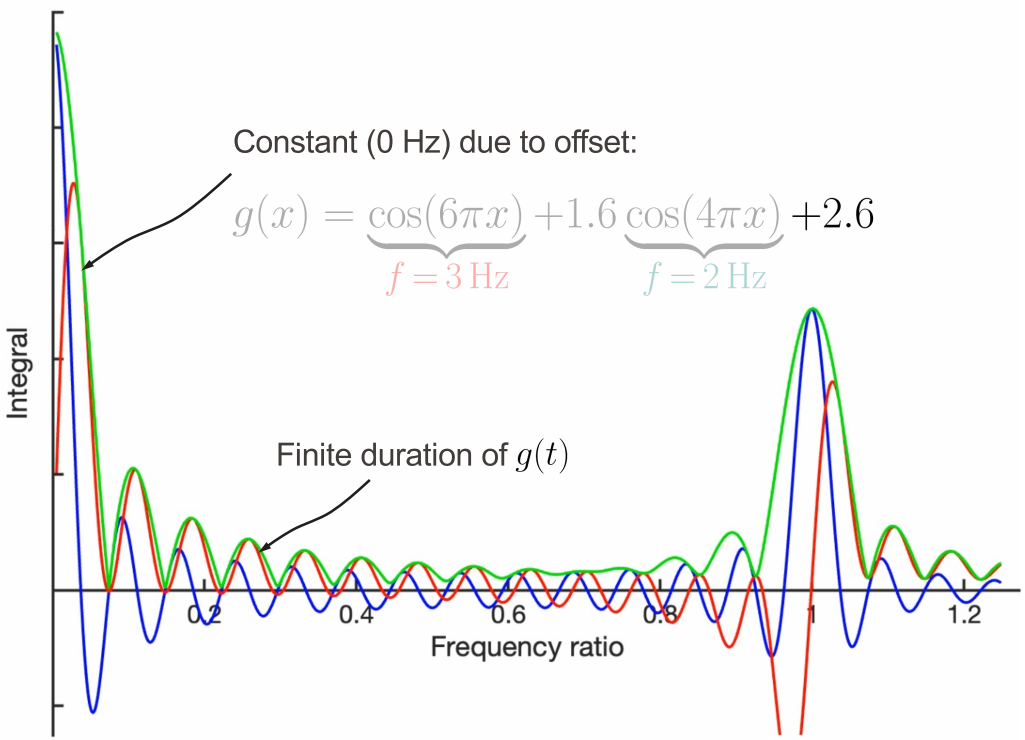


Also for nonperiodic functions…

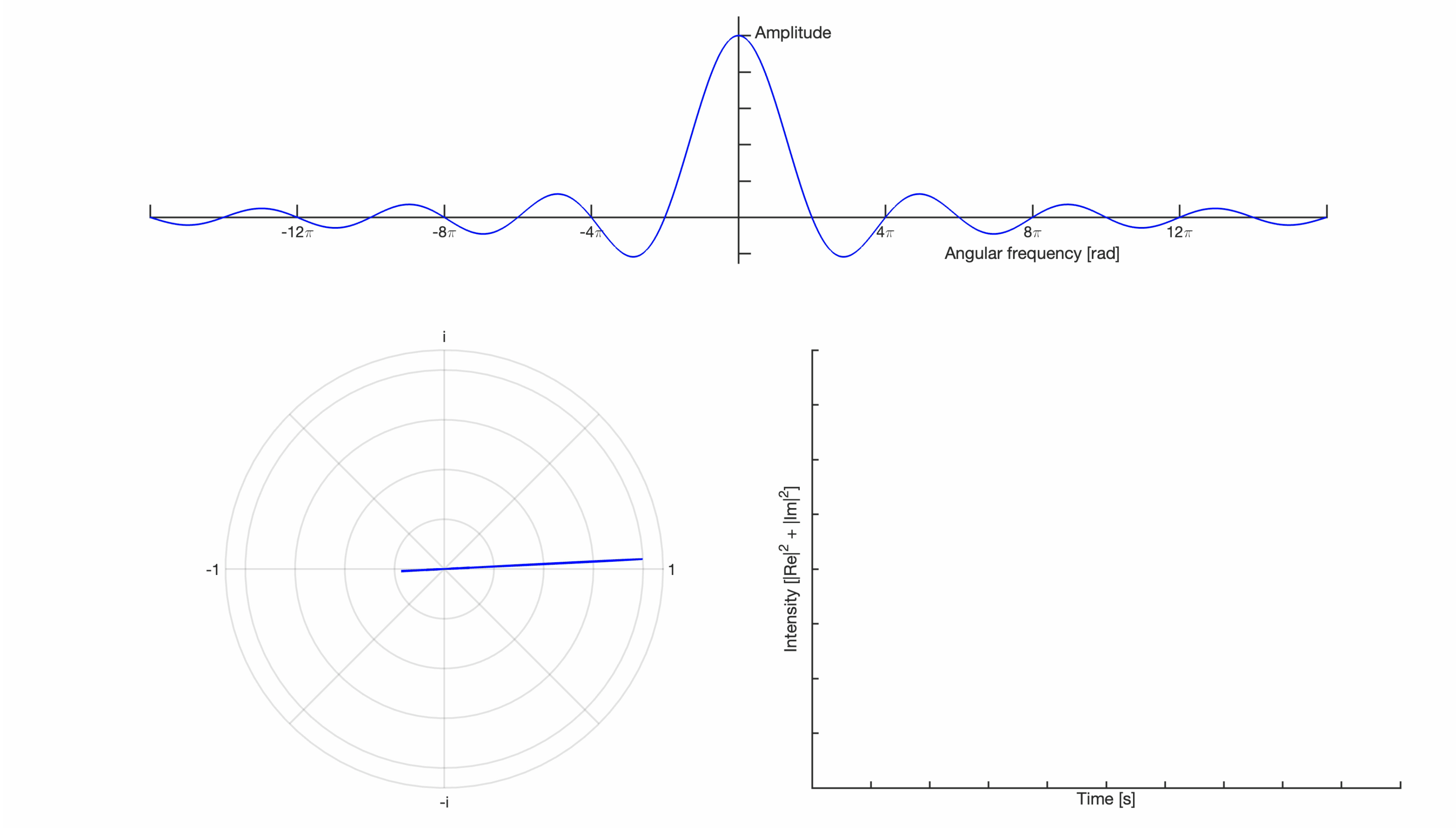


$$\left(\frac{\sin(\pi x/a)}{\pi x/a}\right)^2$$

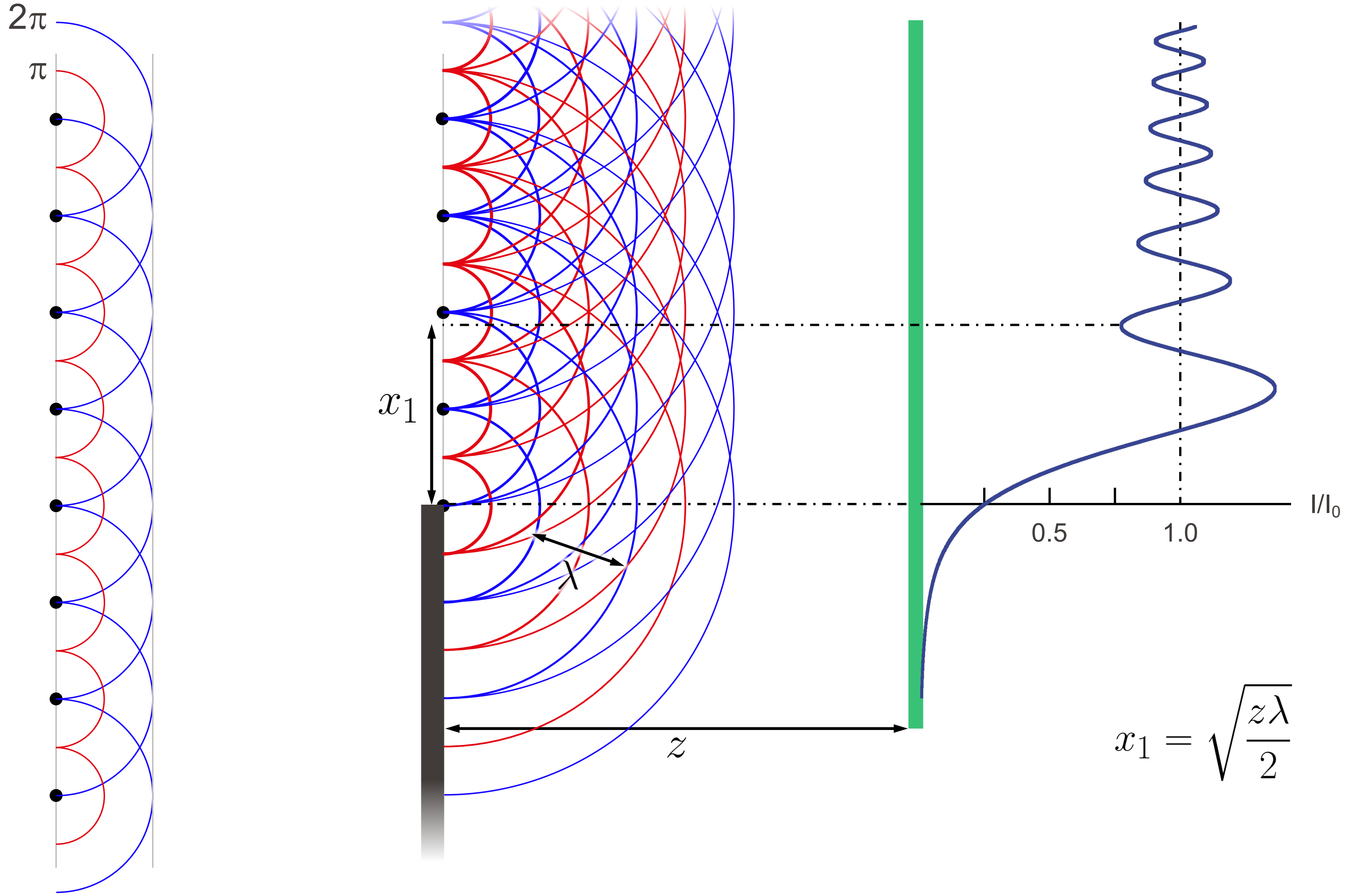
How does a Fourier transform work?



And for completeness, inverse FTs

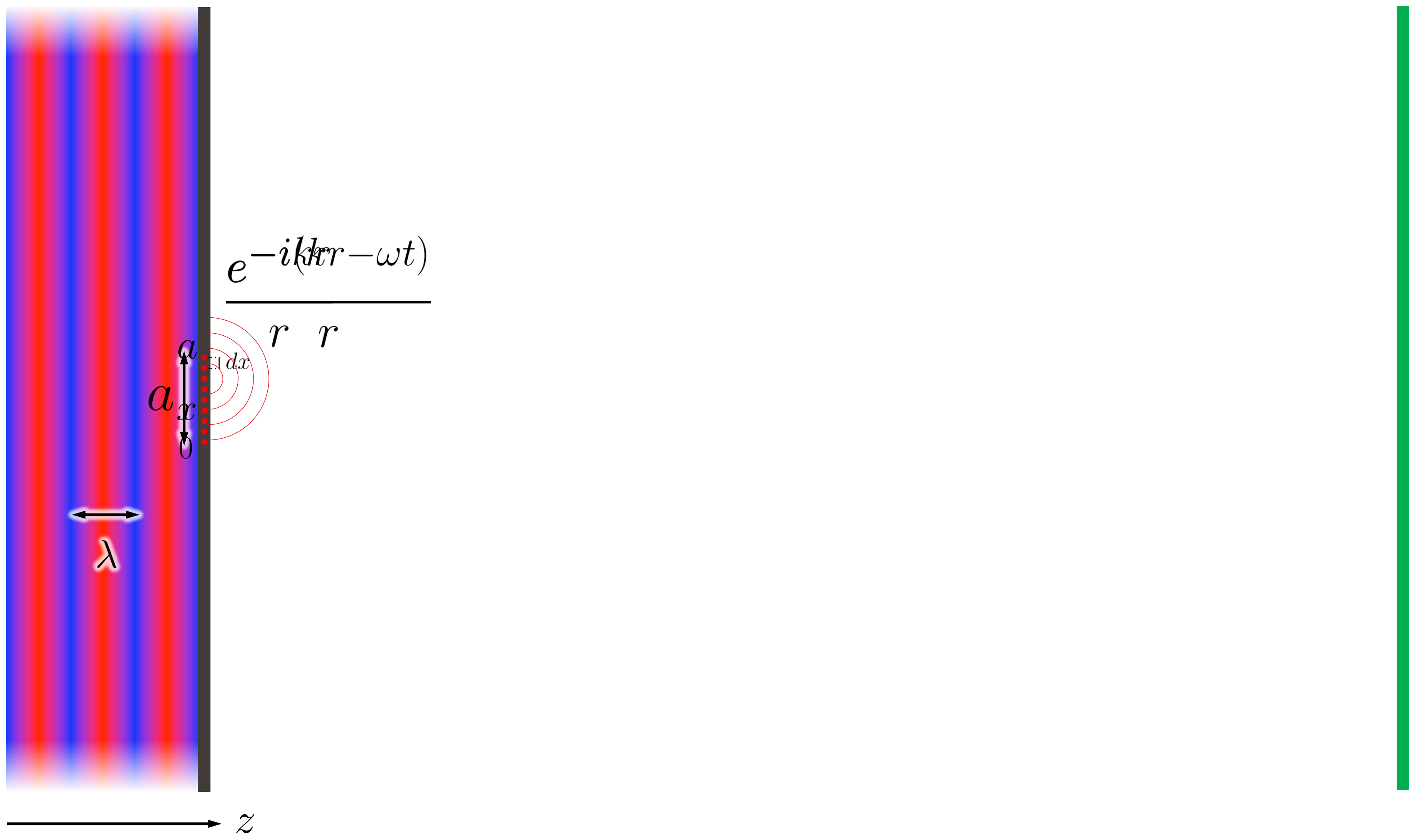


Huygens' construction

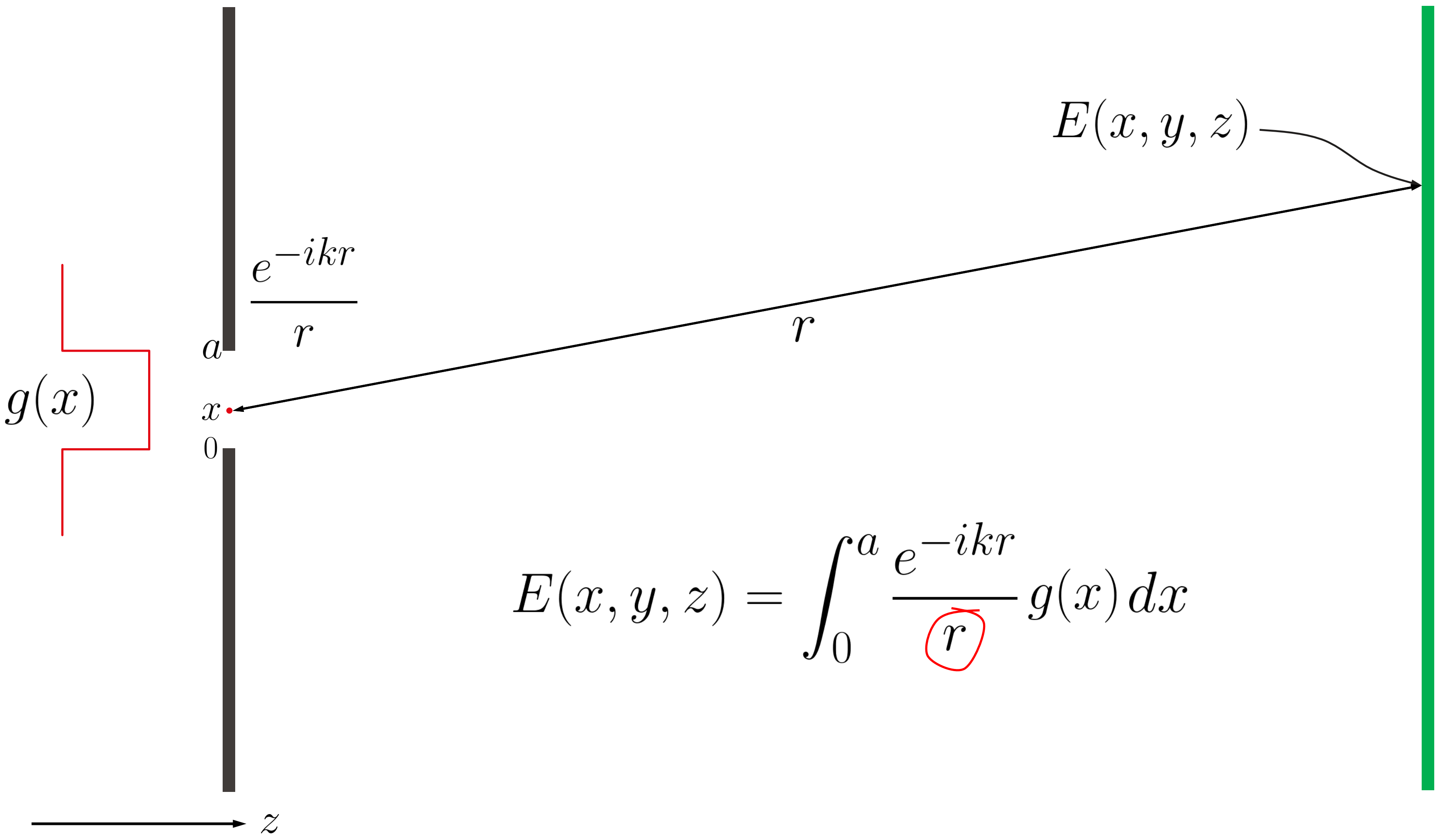


$$x_1 = \sqrt{\frac{z\lambda}{2}}$$

Fraunhofer diffraction – preliminary considerations

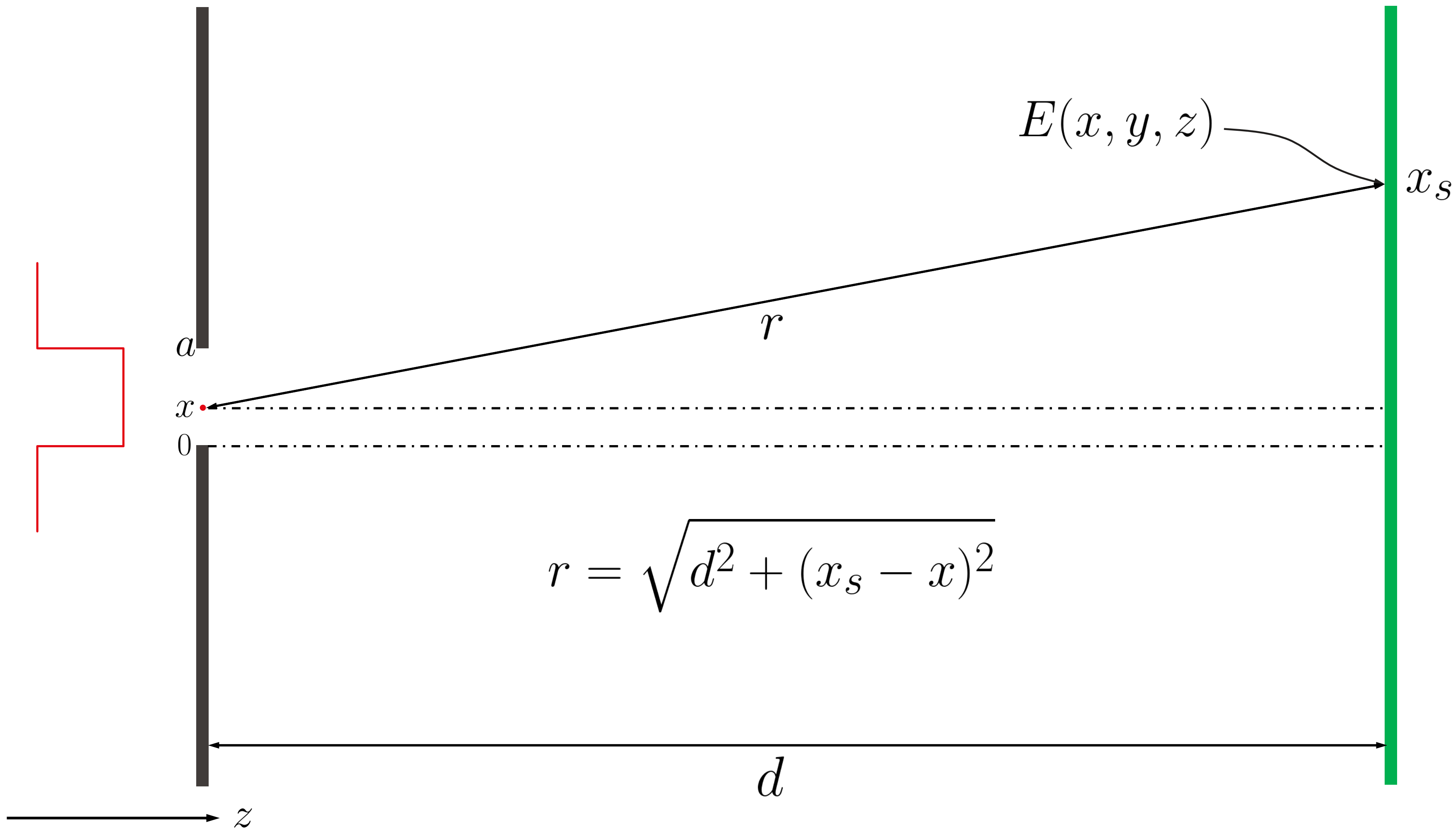


Fraunhofer diffraction – preliminary considerations

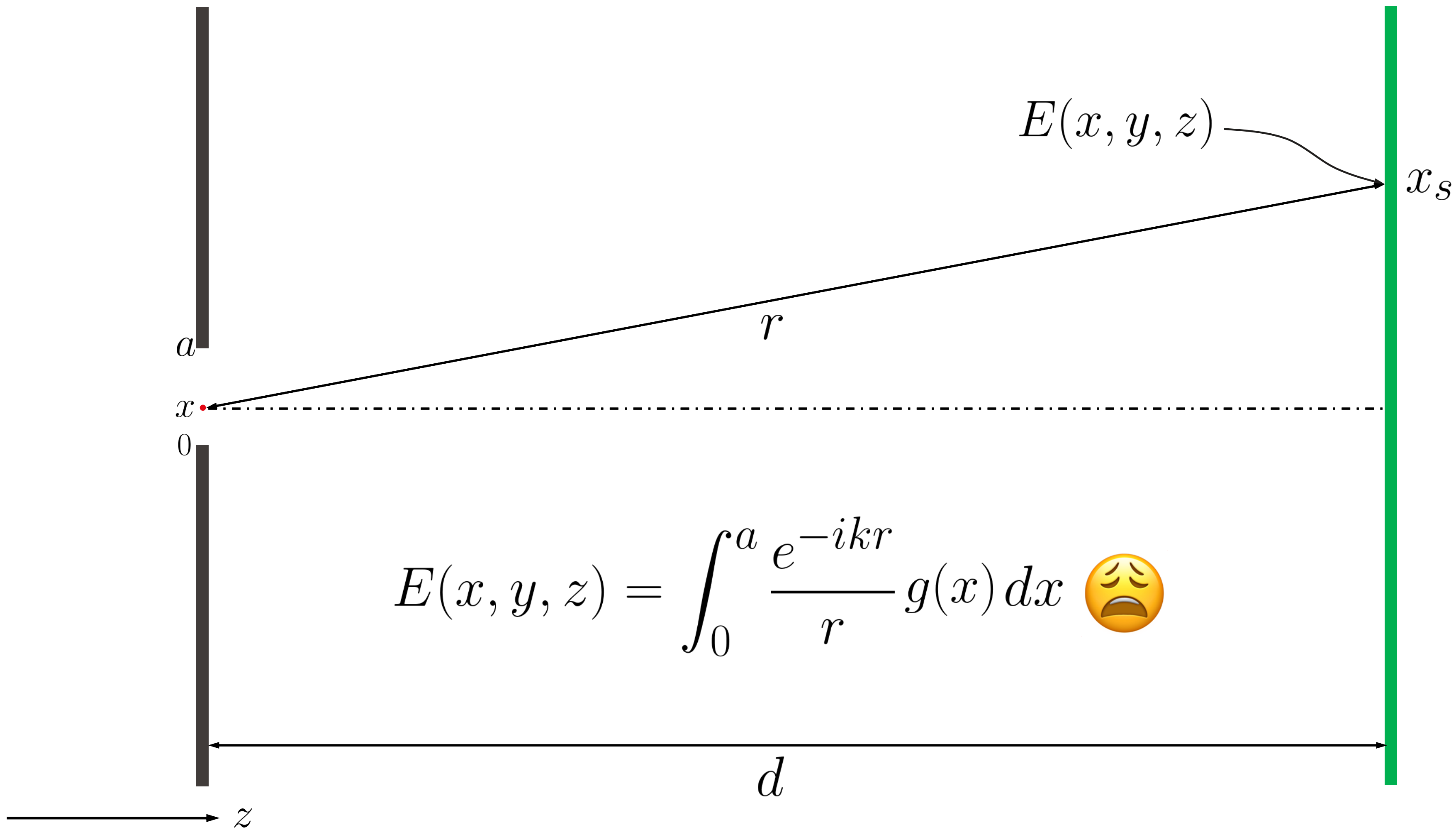


$$E(x,y,z) = \int_0^a \frac{e^{-ikr}}{r} g(x)\,dx$$

Fraunhofer diffraction – preliminary considerations

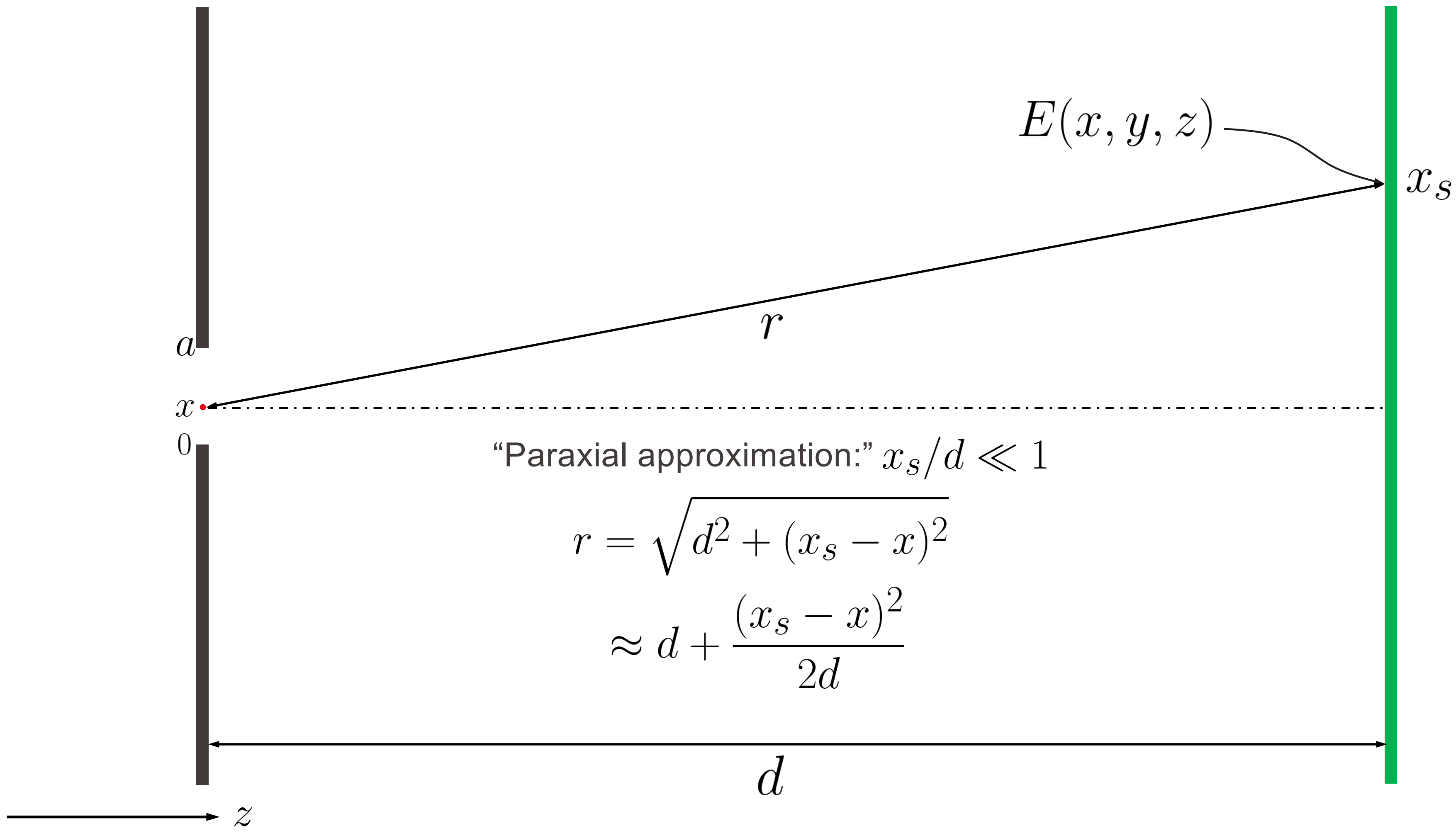


Fraunhofer diffraction – preliminary considerations



$$E(x, y, z) = \int_0^a \frac{e^{-ikr}}{r} g(x)\, dx$$ 😩

Fraunhofer diffraction – simplification 1



"Paraxial approximation:" $x_s/d \ll 1$

$$r = \sqrt{d^2 + (x_s - x)^2}$$

$$\approx d + \frac{(x_s - x)^2}{2d}$$

Fraunhofer diffraction – simplification 1

- Plug $r \approx d + \frac{(x_s - x)^2}{2d}$ into our expression for $E(x,y,z) = \int_0^a \frac{e^{-ikr}}{r} g(x)\,dx$

$$E(x,y,z) \approx \int_0^a \frac{e^{-ik\left(d+\frac{(x_s-x)^2}{2d}\right)}}{d + \frac{(x_s-x)^2}{2d}} g(x)dx \qquad k\frac{(x_s-x)^2}{2d} \not\ll 1$$

$$\approx \frac{e^{-ikd}}{d}\int_0^a e^{-ik\frac{(x_s-x)^2}{2d}} g(x)dx$$

Fraunhofer diffraction – simplification 2

- Now expand

$$k\frac{(x_s - x)^2}{2d} = \frac{kx_s^2}{2d} + \frac{kx^2}{2d} - \frac{kx_s x}{d}$$

Constant for a given x_s and d

Under what conditions can we ignore this?

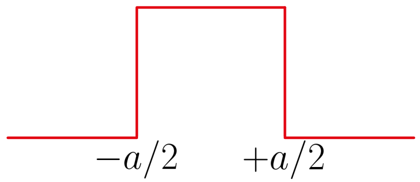
$$\Rightarrow E(x_s, d) \approx \frac{e^{-ikd}}{d} e^{-ikx_s^2/2d} \int_{-a/2}^{a/2} e^{ikx_s x/d}\, g(x)\, dx$$

- Let the aperture be between $\pm a/2 \Rightarrow |x| \leq a/2$

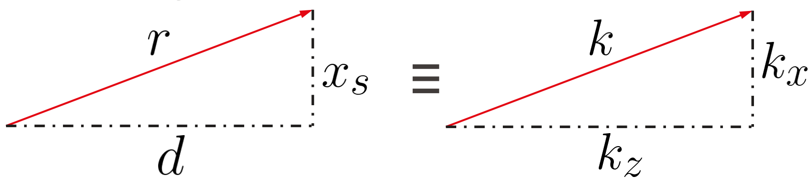
$ka^2/8d = \pi a^2/4\lambda d \ll 1$?

- Fresnel number, $F = a^2/4\lambda d$

$\Rightarrow \pi F \ll 1$



- Similar triangles:

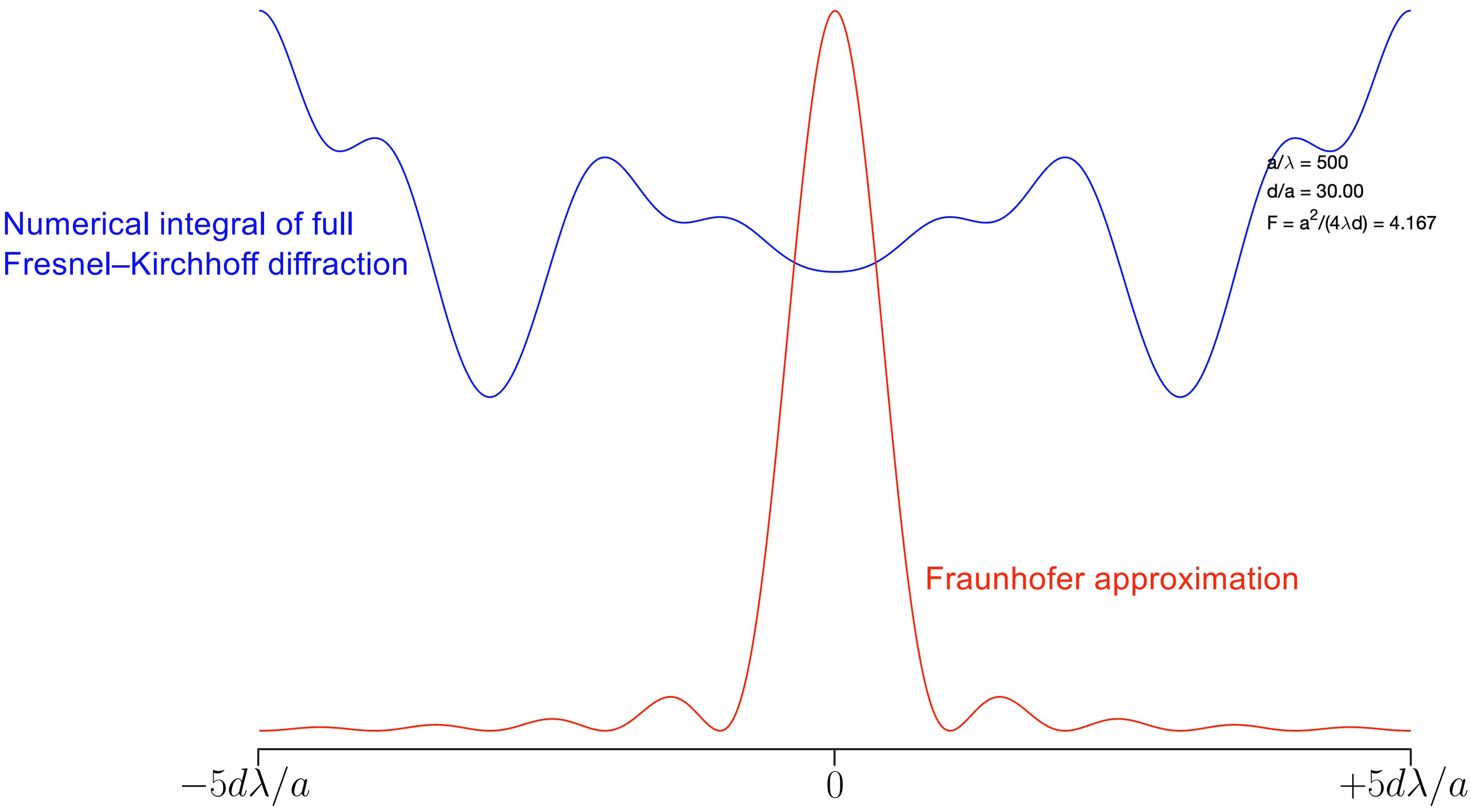


$$\frac{x_s}{d} \approx \frac{k_x}{k} \Rightarrow k_x \approx \frac{kx_s}{d}$$

$$\Rightarrow E(x_s, d) \approx \frac{e^{-ikd}}{d} e^{-ikx_s^2/2d} \underbrace{\int_{-a/2}^{a/2} e^{ikx_x x/d}\, g(x)\, dx}_{\mathcal{F}\{g(x)\}}$$

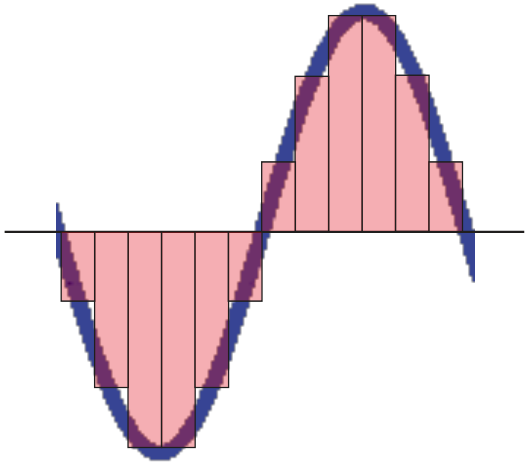
Whatever!

From Fresnel to Fraunhofer



Fraunhofer diffraction = Fourier transform

- Any object can be recreated as a sum of (infinitely narrow) box functions

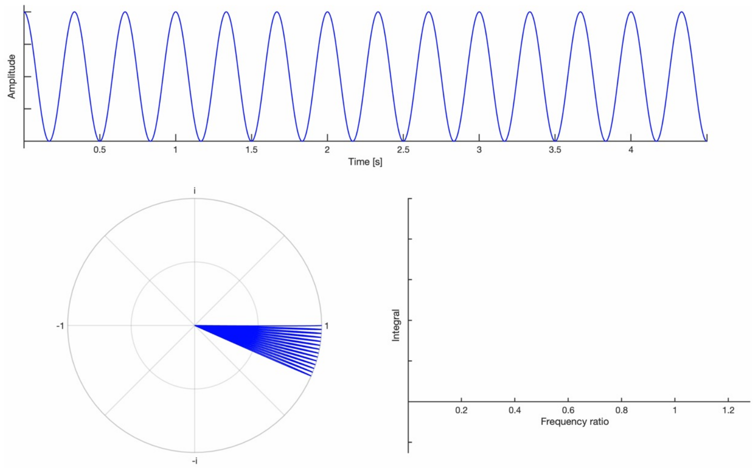


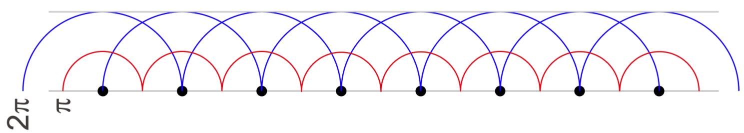
$$\mathcal{F}(a+b) = \mathcal{F}(a) + \mathcal{F}(b)$$

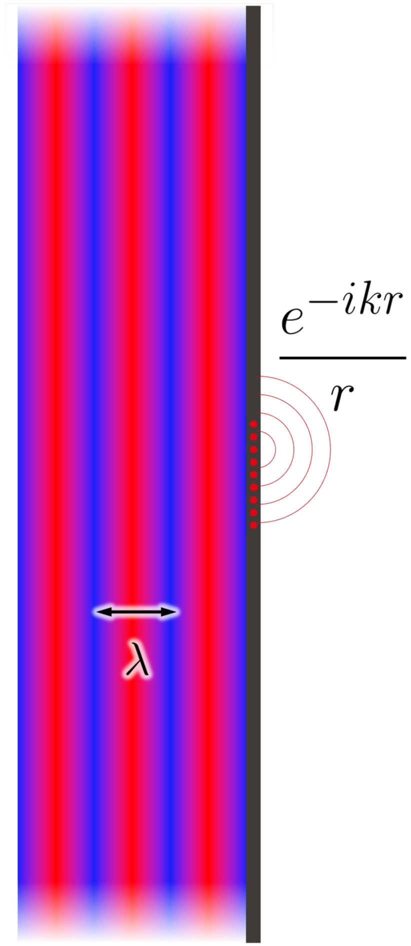
$$\Rightarrow E(x,y,z) = \mathcal{F}\{g(x)\} \text{ for any } g(x)$$

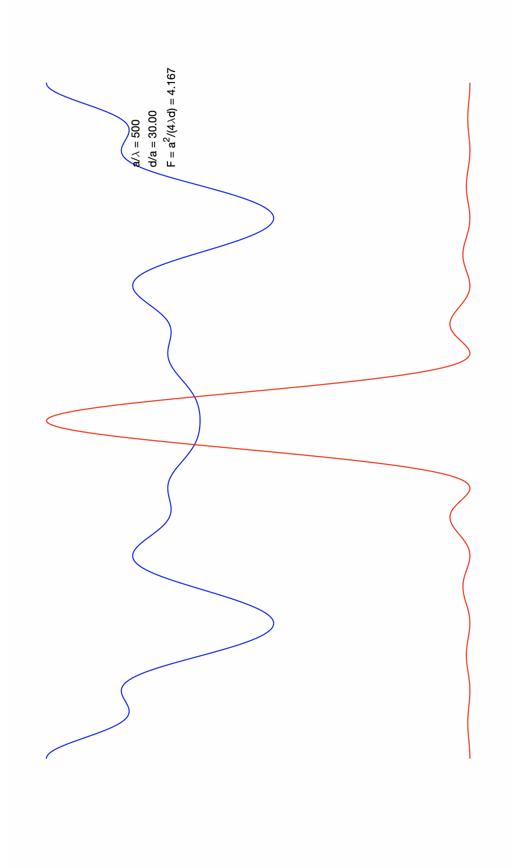
Summary of FTs and diffraction regimes

$$\mathcal{F}\{g(x)\} = \int_a^b g(x)\, e^{-ikx}\, dx$$



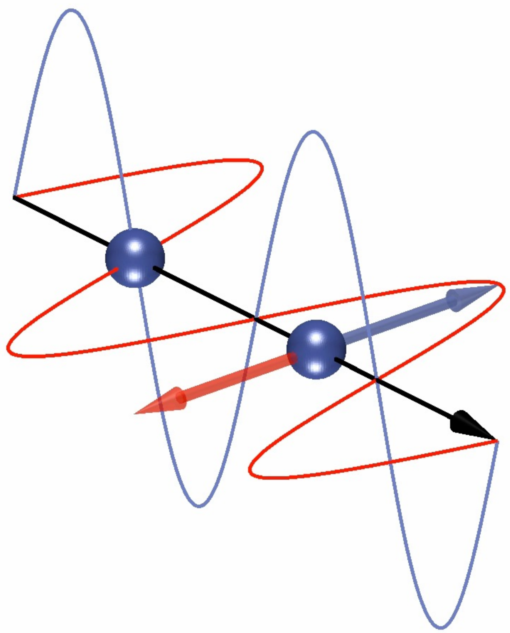






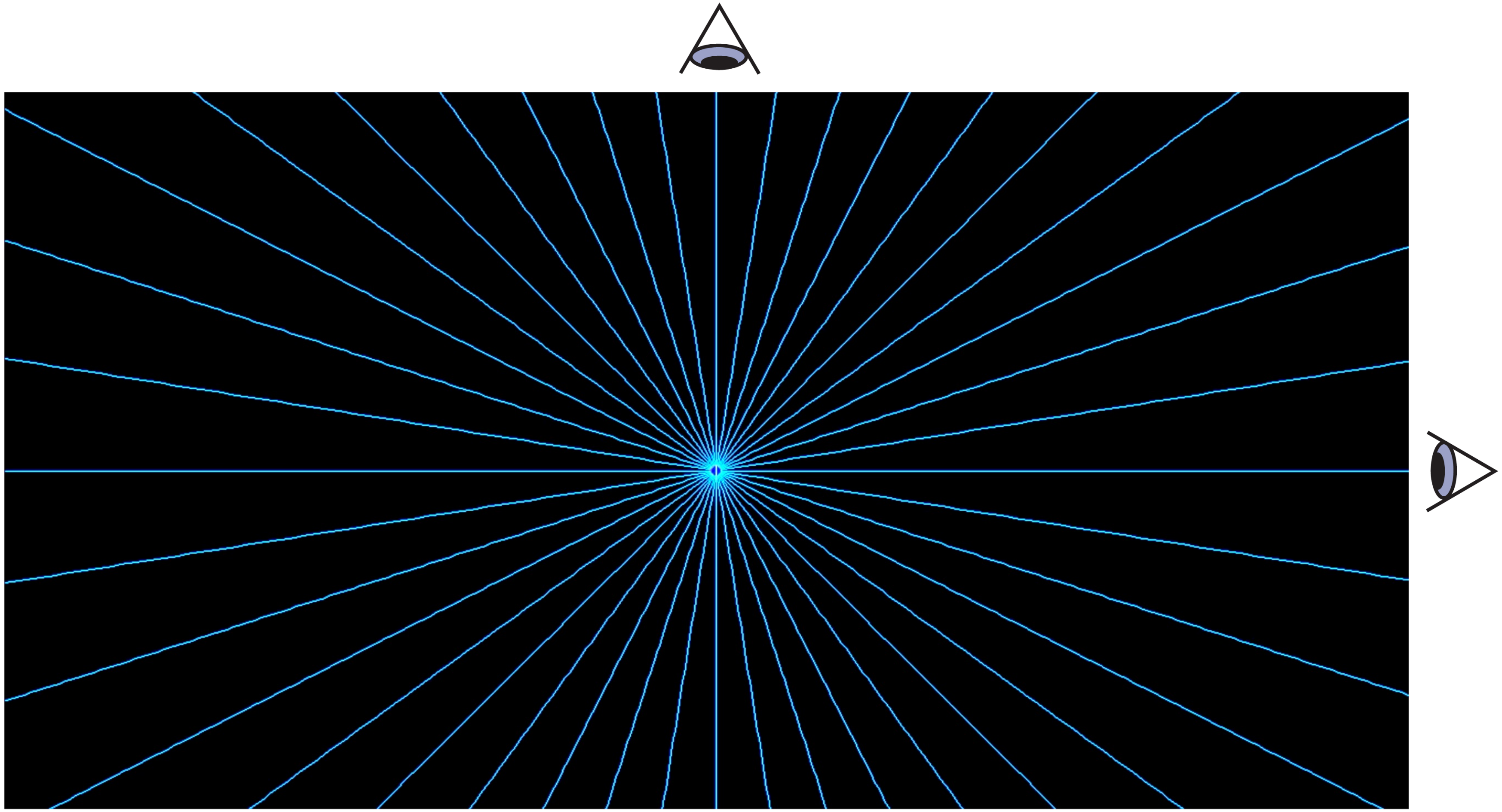
Dipole radiation and elastic scattering by electrons

Electric and magnetic forces



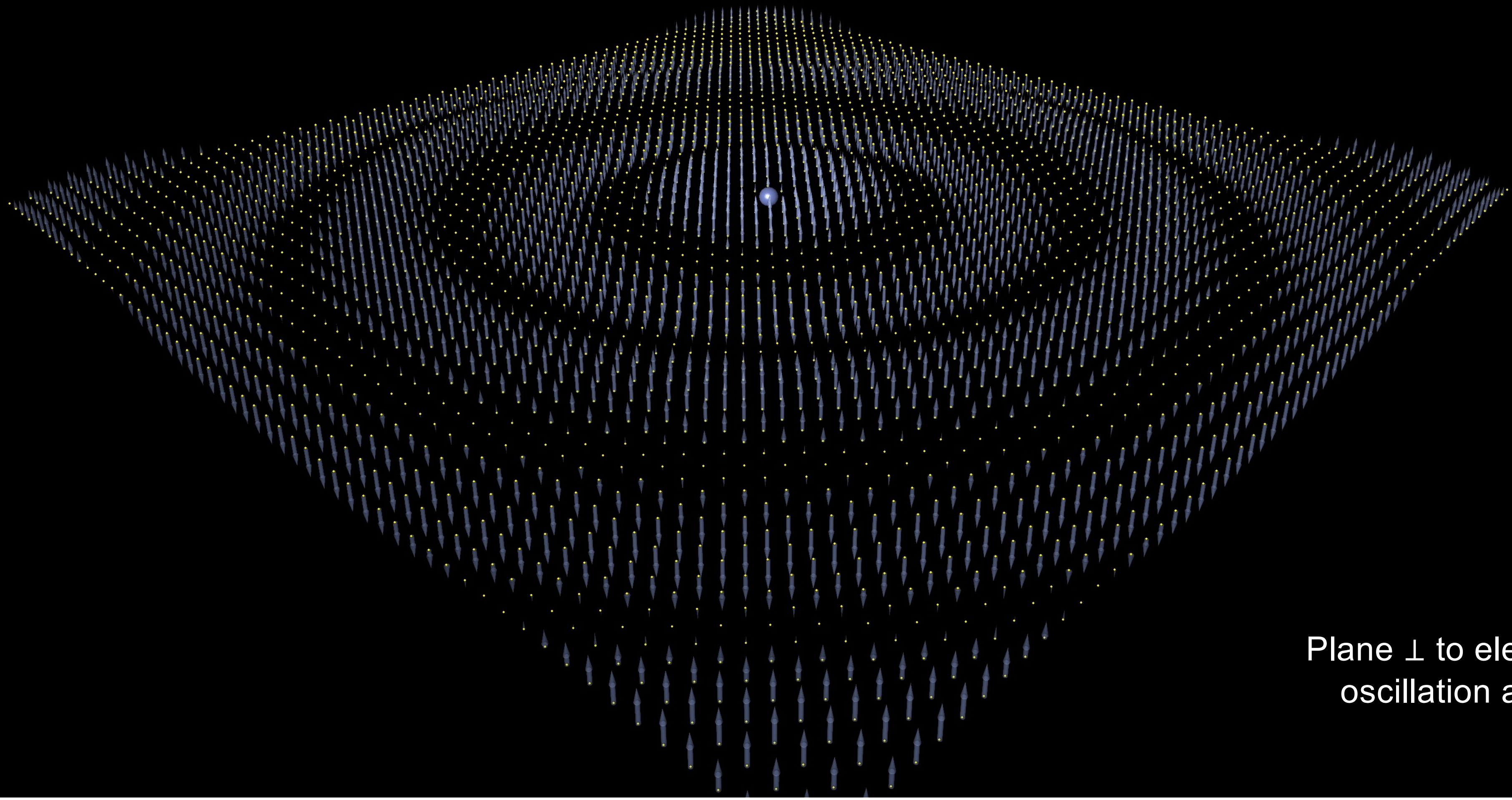
- Incident electromagnetic radiation with
  - Electric field $\vec{E}$
  - Magnetic field $\vec{B}$
- Forces on electron
  - $\vec{F}_E = -e\vec{E} = -eE_0 \cos(kz - \omega t)$
  - $\vec{F}_B = e\vec{v} \times \vec{B} = e|\vec{v}|\,|\vec{B}|$
- From classical EM theory: $|\vec{B}| = \frac{|\vec{E}|}{c}$
  - $\Rightarrow \frac{|\vec{F}_B|}{|\vec{F}_E|} = \frac{v}{c}$
  - Magnetic forces only significant for relativistic electrons

Driving an electron with electromagnetic radiation



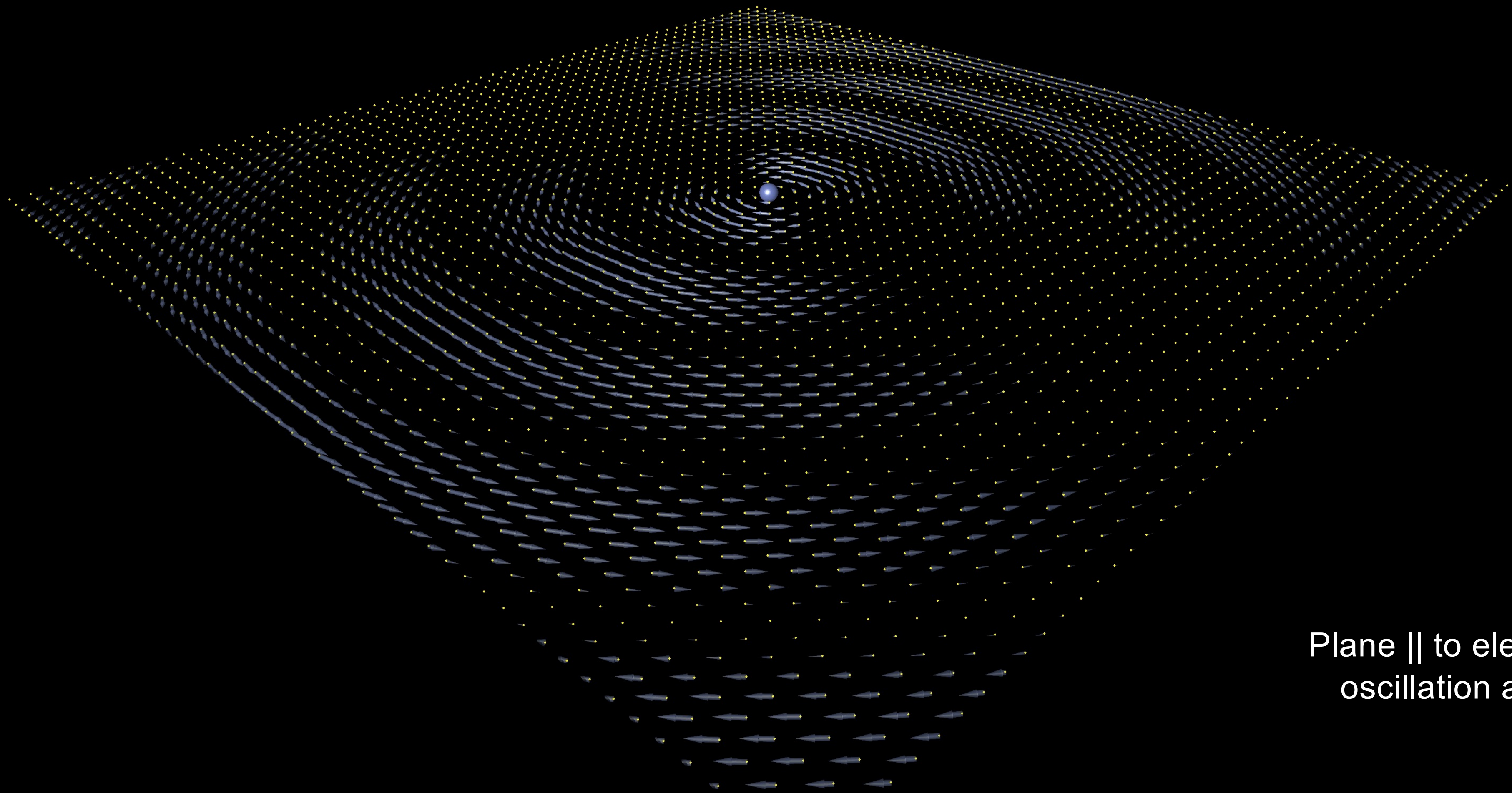
http://www.shintakelab.com/en/enEducationalSoft.htm

$$E(\vec{r}, t) = \frac{-q}{4\pi\epsilon_0 c^2} \frac{1}{|r|} a_\perp(t - |r|/c)$$



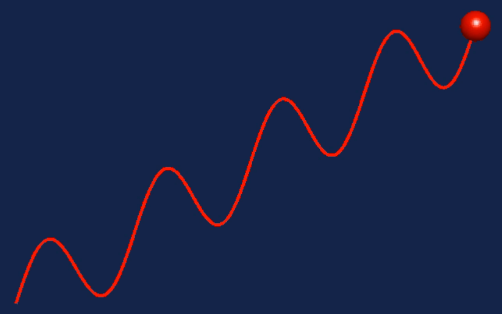
Plane ⊥ to electron oscillation axis

$$E(\vec{r},t) = \frac{-q}{4\pi\epsilon_0 c^2}\frac{1}{|r|}a_\perp(t-|r|/c)$$



Plane || to electron oscillation axis

… and in 3D, dipole radiation

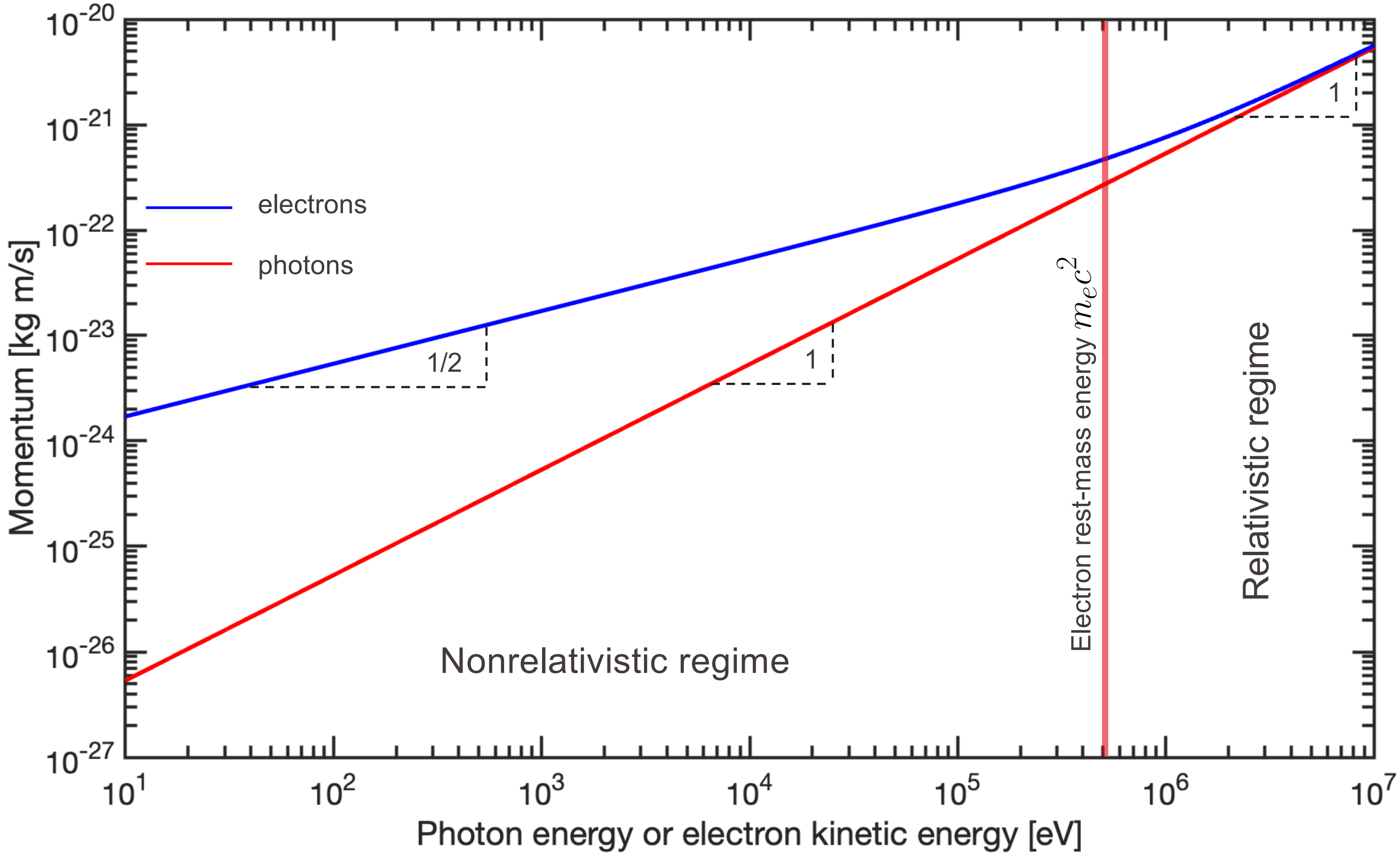


Compton and Thomson scattering

Energy and momenta of electrons and photons

- Photons
  - Energy: $E_p = hc/\lambda_p = h\nu$
  - Momentum: $p_p = h/\lambda_p \propto E_p$
- Electrons
  - Total energy: $E_{e,\text{tot}} = \dfrac{m_e c^2}{\sqrt{1 - v^2/c^2}} = \gamma m_e c^2$
  - Kinetic energy: $E_{e,K} = \gamma m_e c^2 - m_e c^2 = (\gamma - 1) m_e c^2$
  - Momentum: $p_e = \gamma m_e v$
    - Limit $v \ll c: \;\; p_e \approx m_e v \propto (E_{e,K})^{1/2}$
    - Limit $v \sim c: \;\; p_e \approx E_{e,\text{tot}}/c \approx E_{e,K}/c$

Energy and momenta of electrons and photons



The classical electron radius, or Thomson length

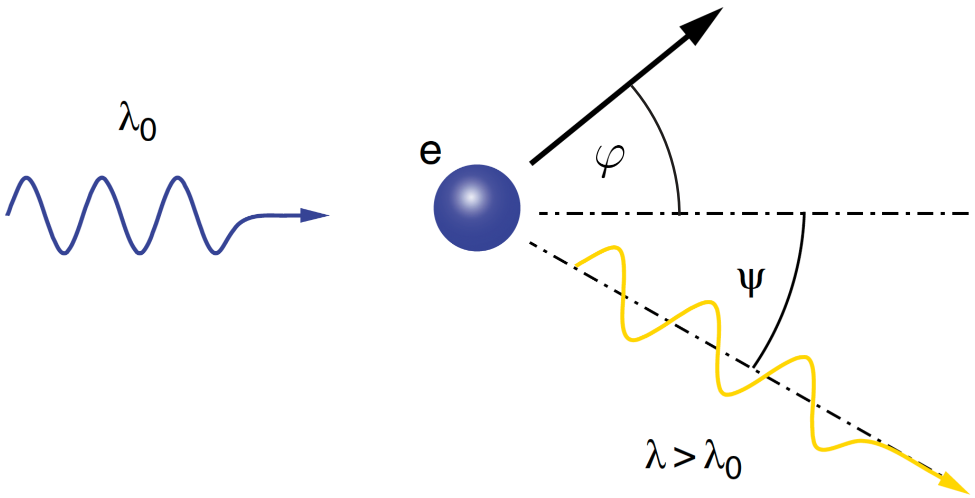
- Equate the electrostatic potential of an electron at a distance r_0 with its rest-mass energy, $m_e c^2$

$$\Rightarrow \frac{e^2}{4\pi\epsilon_0 r_0} = m_e c^2$$

$$\Rightarrow r_0 = \frac{e^2}{4\pi\epsilon_0 m_e c^2} = 2.82 \times 10^{-5}\ \text{Å}$$

- This does not imply the radius of an electron is, in reality, this size (a free electron is, as far as we can tell, infinitely small), but is useful for defining interaction lengths, such as we will see for Compton and Thomson scattering

Scattering of a photon by an electron



- Conservation of energy and momentum
  - Photon loses energy and momentum
  - Electron recoils and gains energy lost by photon
- Derivation provided e.g., https://en.wikipedia.org/wiki/Compton_scattering

$$\frac{h\nu_0}{h\nu} = \frac{k_0}{k} = \frac{\lambda}{\lambda_0} = 1 + \frac{\lambda_C}{\lambda_0}(1 - \cos\psi) \quad \left(\lambda_C = \frac{h}{m_e c} = 2.43 \times 10^{-2}\,\text{Å}\right)$$

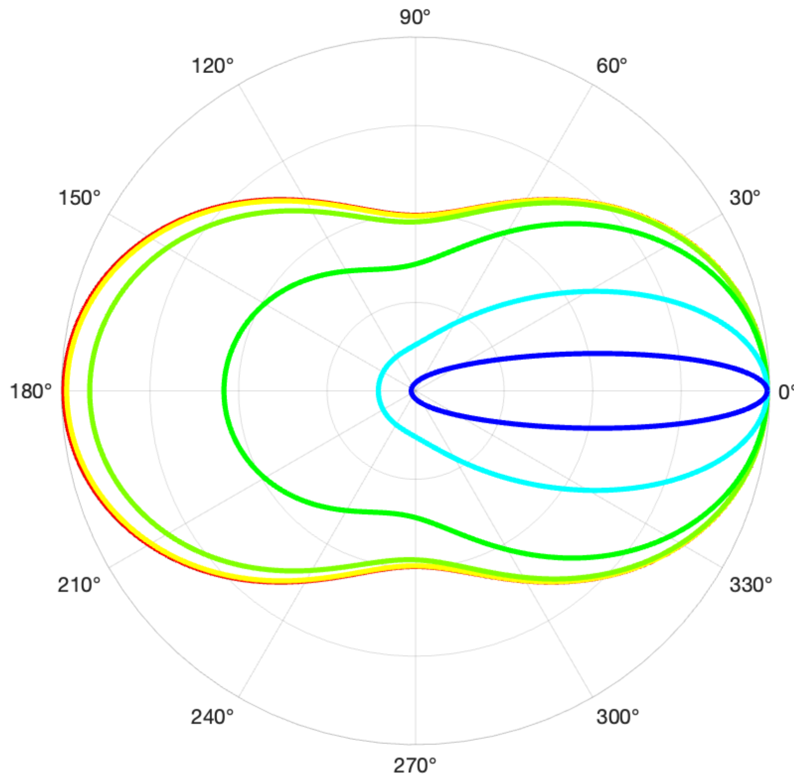
$$\cot\varphi = \left(1 + \frac{h\nu_0}{m_e c^2}\right)\tan\left(\frac{\psi}{2}\right)$$

- $\lambda_0 \gg \lambda_C$: low-energy regime = Thomson scattering
- $\lambda_0 \lesssim \lambda_C$: higher-energy regime $\gtrsim$ 200 keV = Compton scattering

Klein-Nishina equation

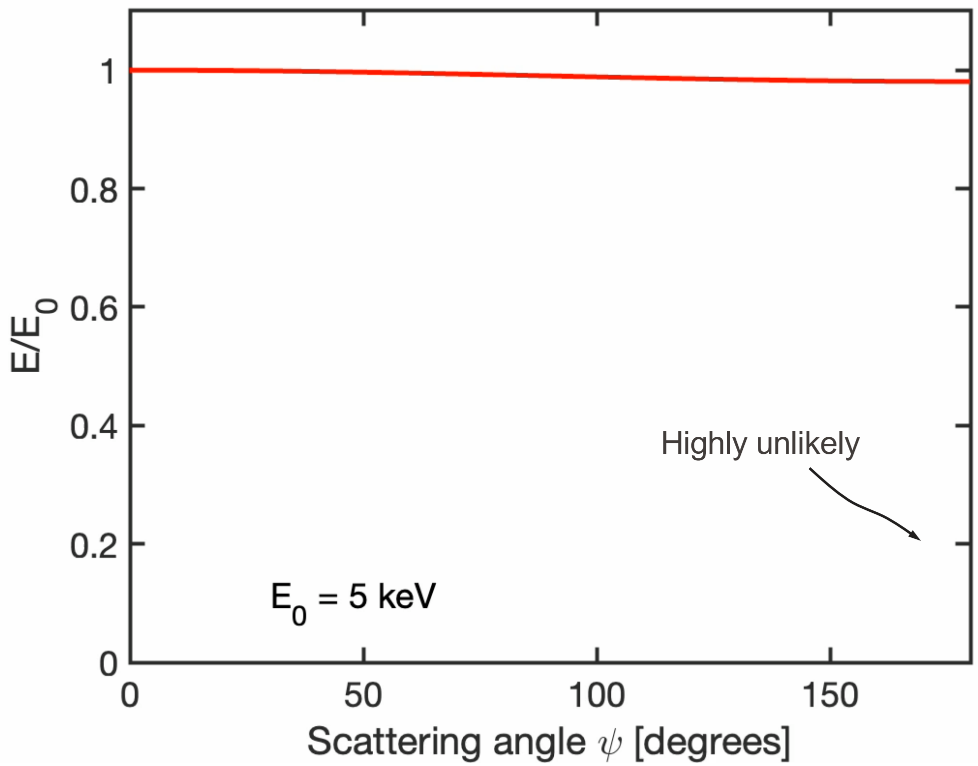
$$\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2}\left(\frac{\lambda_0}{\lambda}\right)^2 \left[\frac{\lambda_0}{\lambda} + \frac{\lambda}{\lambda_0} - \sin^2\psi\right]$$ (unpolarized)

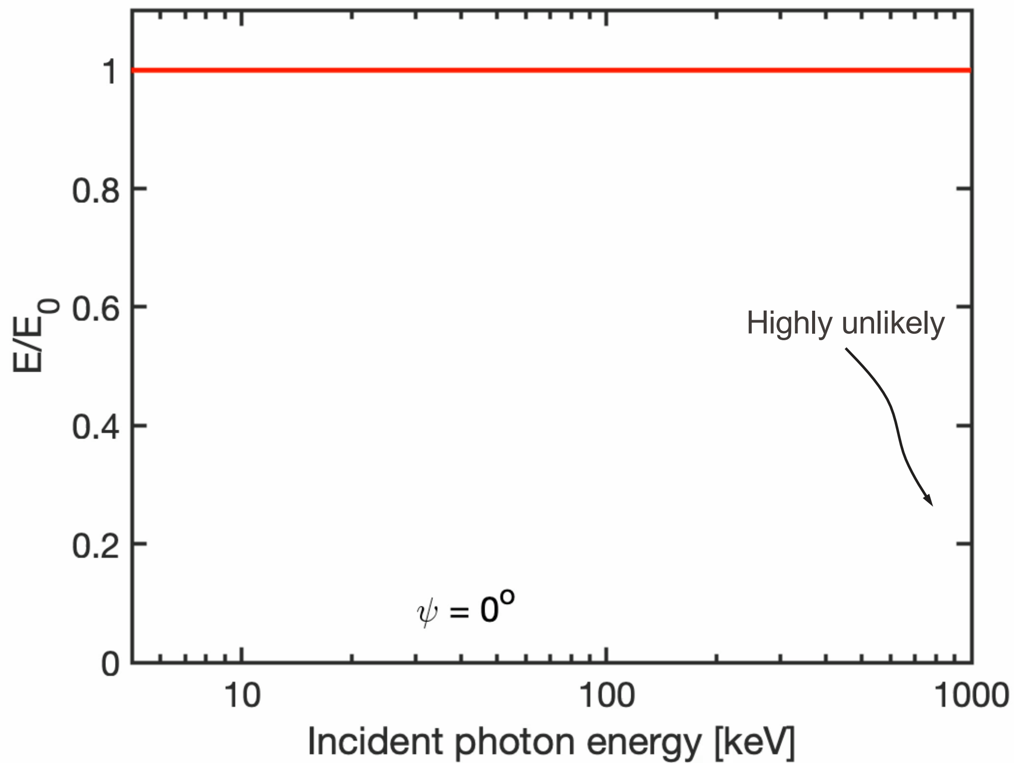
$$\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2}\left(\frac{\lambda_0}{\lambda}\right)^2 \left[\frac{\lambda_0}{\lambda} + \frac{\lambda}{\lambda_0} - 2\sin^2\psi\cos^2\phi\right]$$ (linearly polarized)



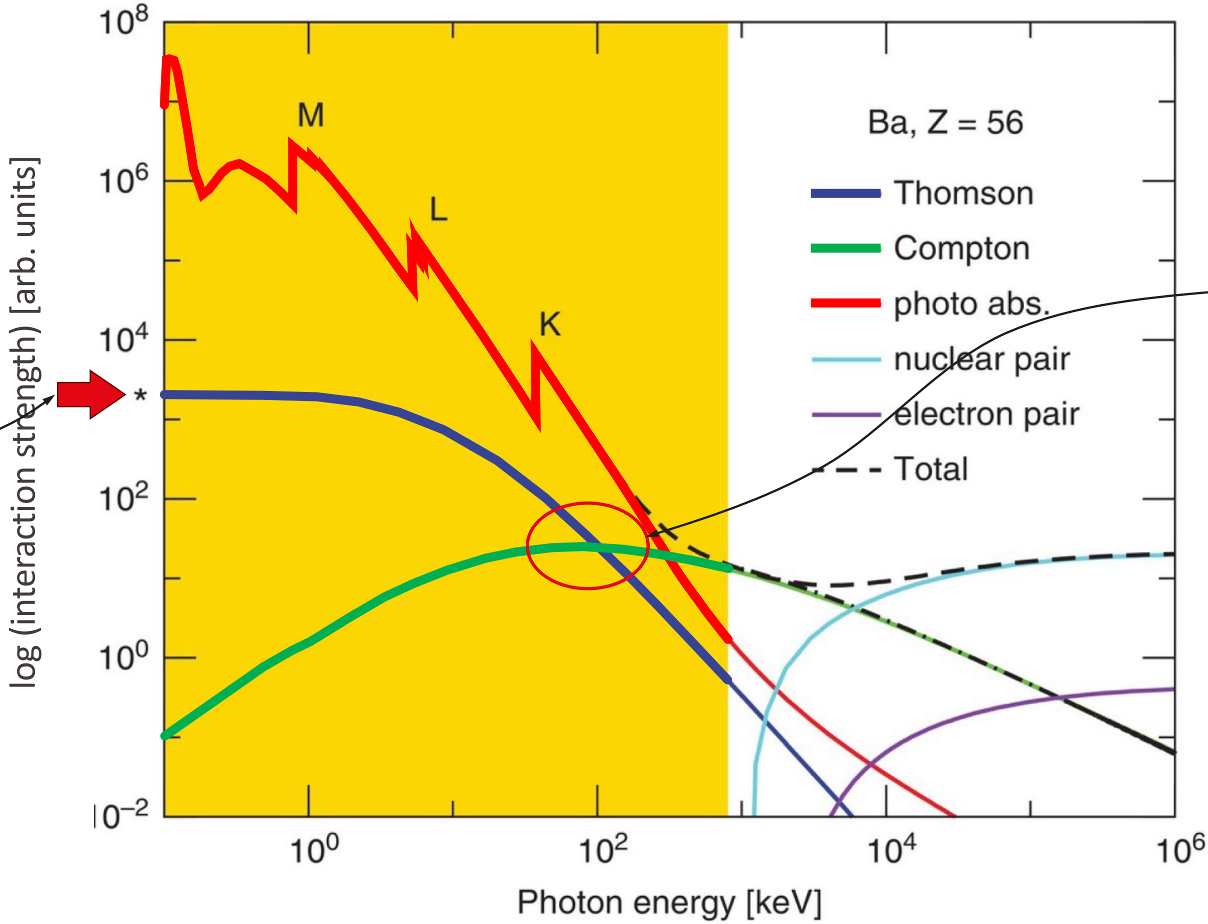
E_0 = 10 eV – 1 MeV (decade steps)

Compton scattering





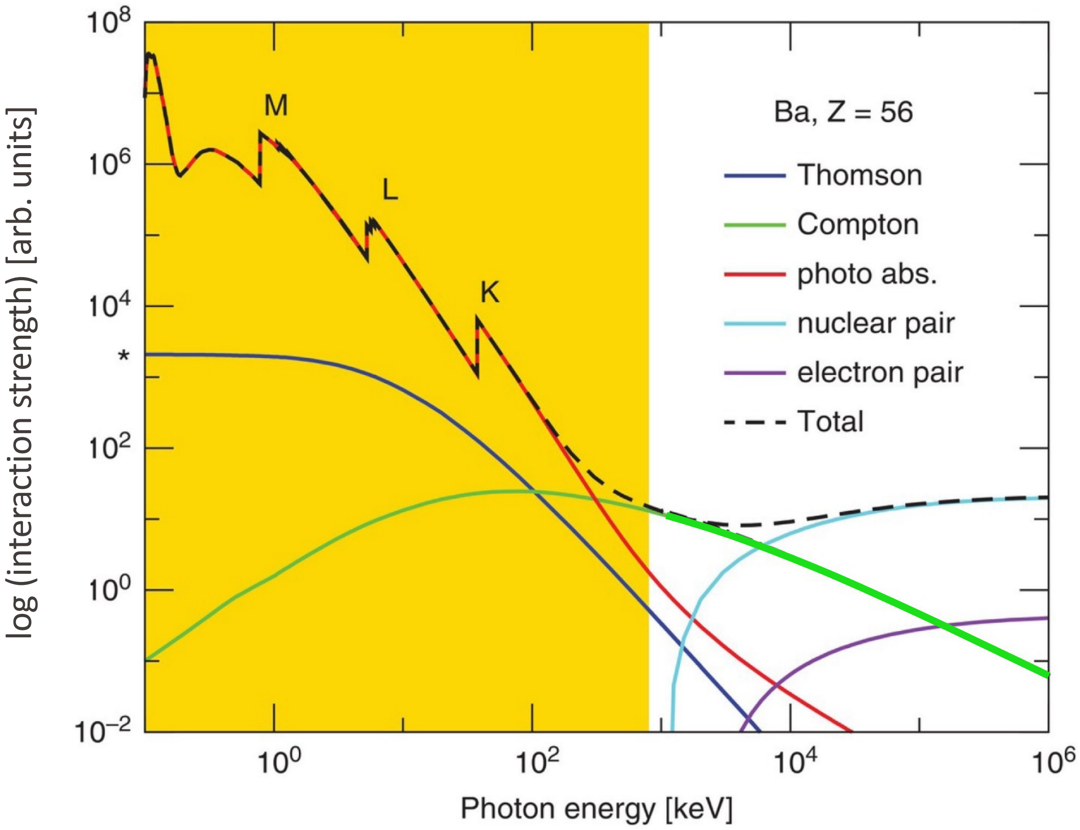
Interaction strengths of UV and x-rays with matter



Low energies: λ ≫ atom ⇒ in-phase scattering (see later)

Electrons in atoms are bound with defined energy levels… A “bit” of energy transfer doesn’t cut it!!

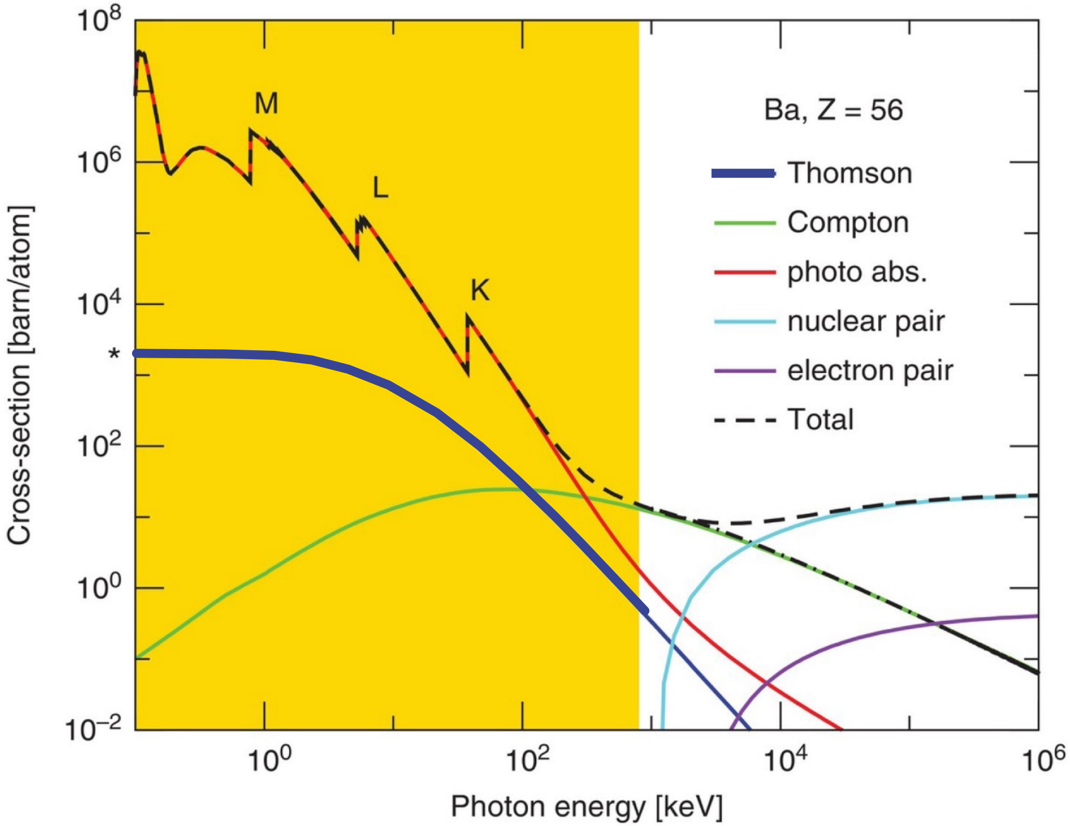
Interaction strengths of UV and x-rays with matter



- Maximum of Compton scattering ~ 100 keV to 1 MeV
  - Lower photon energies: energy imparted to bound electron is insufficient to promote it to either an unbound excited state, or completely eject it into vacuum
    ⇒ atom is left in its ground state: Thomson scattering dominates. Cross-section proportional to Z^2
  - Higher photon energies: electrons escape confines of the atom. Compton cross-section for an atom of atomic number Z approaches

$$\sigma_C \approx \frac{Z\pi r_0^2}{2\zeta}\left[1 + 2\ln(2\zeta)\right]; \quad \zeta = \lambda_C/\lambda_0$$

More on Thomson scattering



- Remember: Thomson length

$$r_0 = \frac{e^2}{4\pi\epsilon_0 m_e c^2} = \boxed{2.82 \times 10^{-5}\ \text{Å}}$$

- Obtain free-electron cross-section by integrating dipole radiation over polar coordinates ϕ and ψ.

Leads to

$$\boxed{\sigma_T = \left(\frac{8\pi}{3}\right) r_0^2 = 0.665\,\text{b}}$$

(1 barn = 10^{-28} m^2)

Important!

The electron is the only important particle describing the interaction of UV light and x-rays with matter

For the remainder of this part of the course, I will ignore Compton scattering and assume only Thomson scattering

Coming up later today…