ECE 535: Introduction to Quantum Sensing

Diffraction and the uncertainty principle

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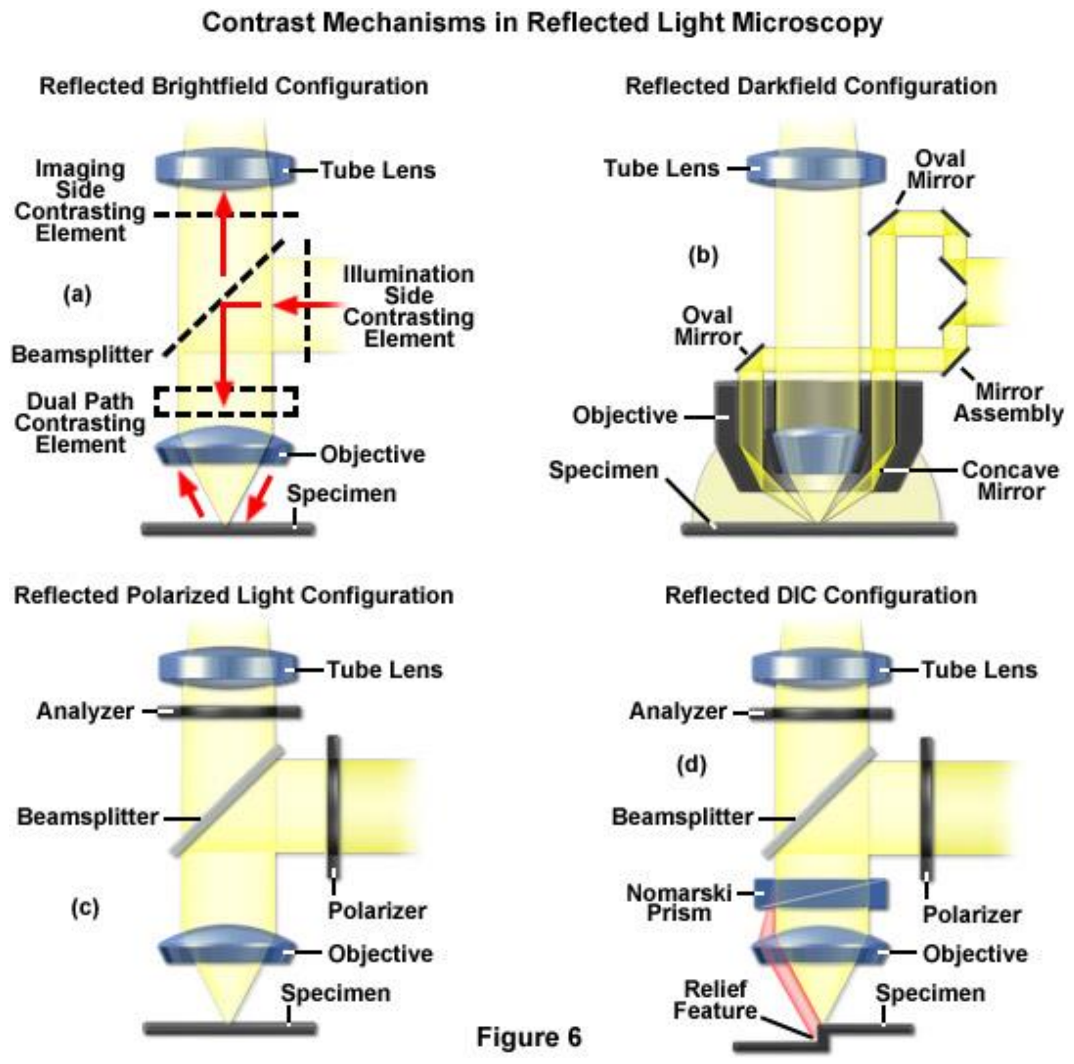
Topics

- Resolution limits in electron and light microscopy
- Diffraction of matter waves
- Defining wave functions
- Uncertainty principle

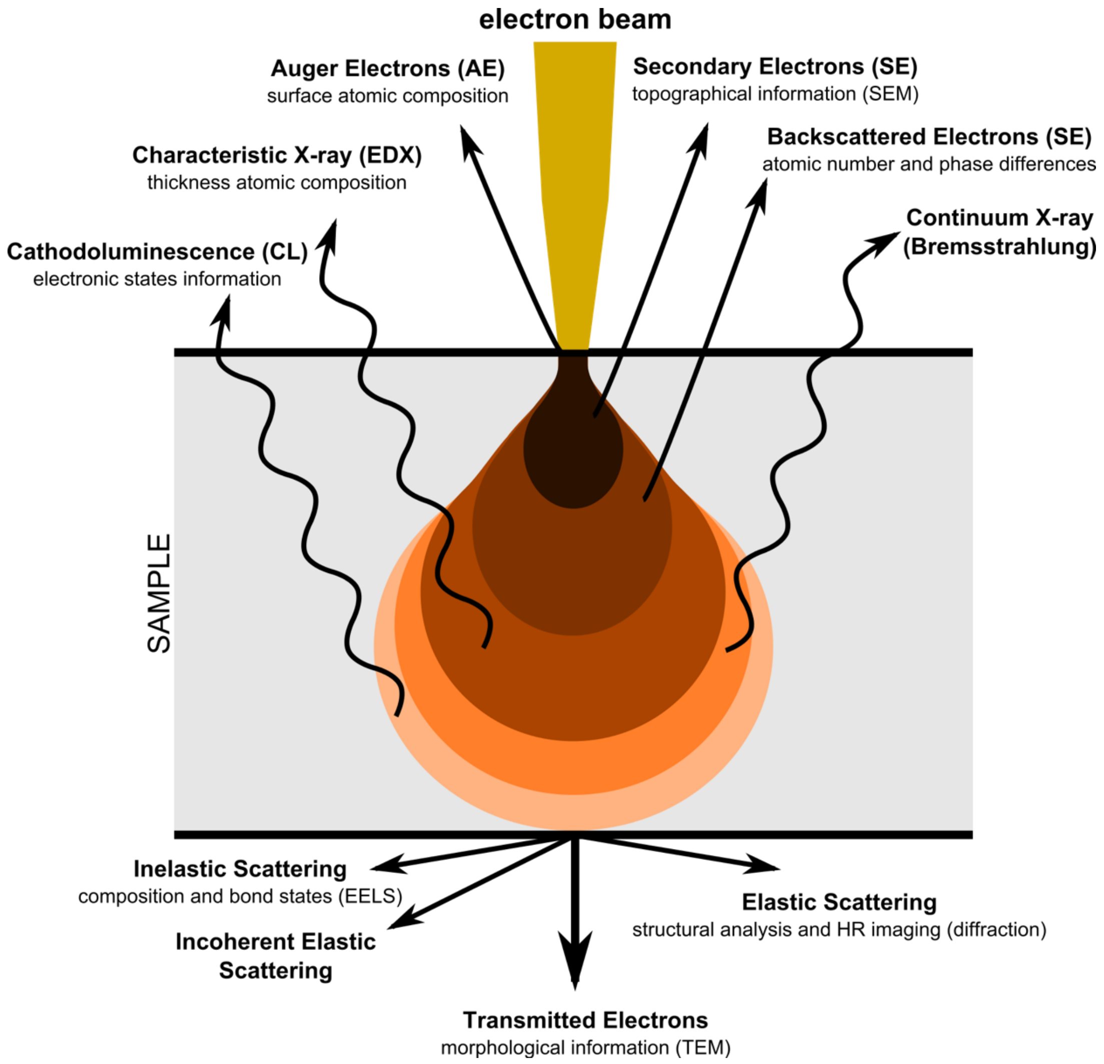
Some examples of microscopy

Reflected light microscopy



Source: ZEISS microscopy

Electron microscopy



Source: Claudionico (Wikipedia)

Microscopy with light and electrons

- Comparison between visible wavelengths and de Broglie wavelengths of electrons

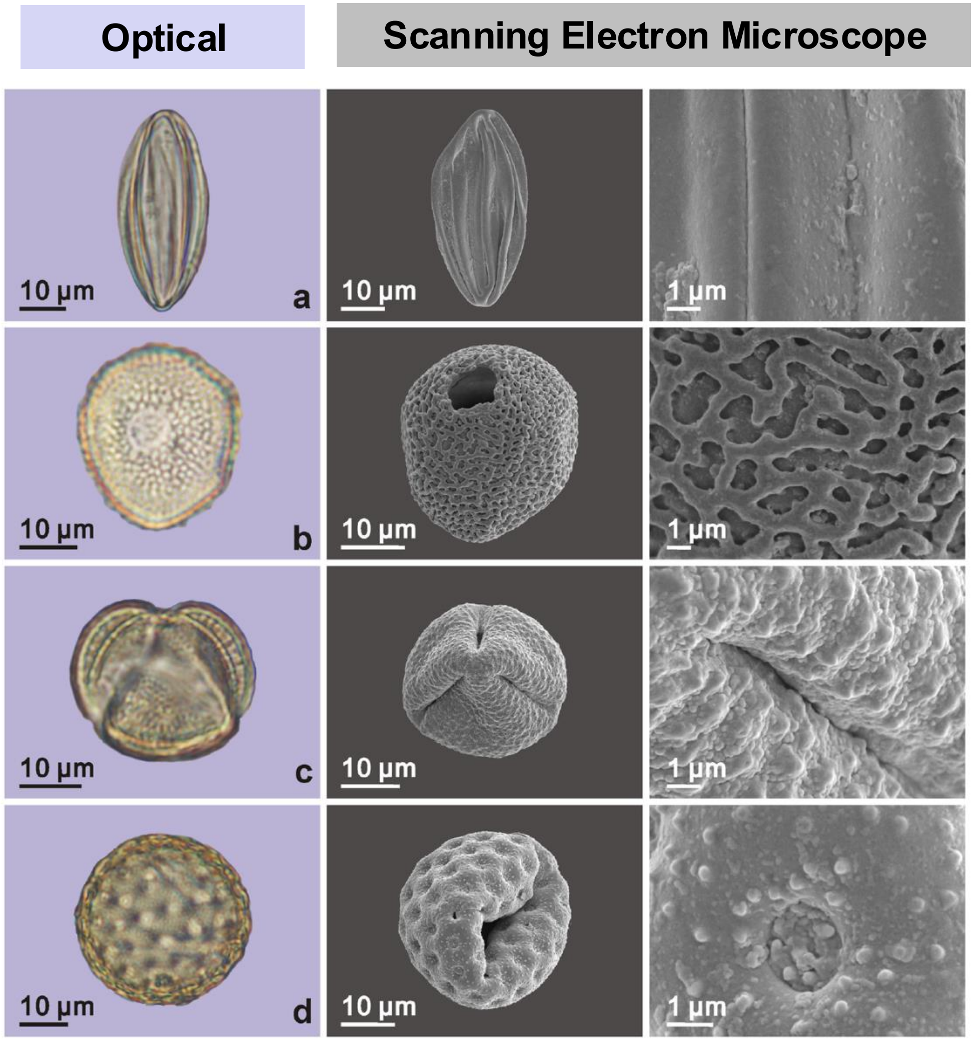
$$\lambda_{visible} \approx 400 - 700\, nm$$

$$\lambda_e = \frac{hc}{\sqrt{E_{kin}^2 + 2E_{kin} m_e c^2}}; m_e c^2 = 0.511\, MeV \text{ for electrons}$$

$$\lambda_e \approx 0.0037\, nm \text{ for 100 keV electrons}$$

- Resolution of an imaging system is ultimately limited by the wavelength of the source (rule of thumb, the best you can do is ~$\lambda/2$) → much better resolution for microscopy and lithography!
  - Reason why electron microscopes still have resolution limits ~ 0.1 nm is due to limitations in electron-optics

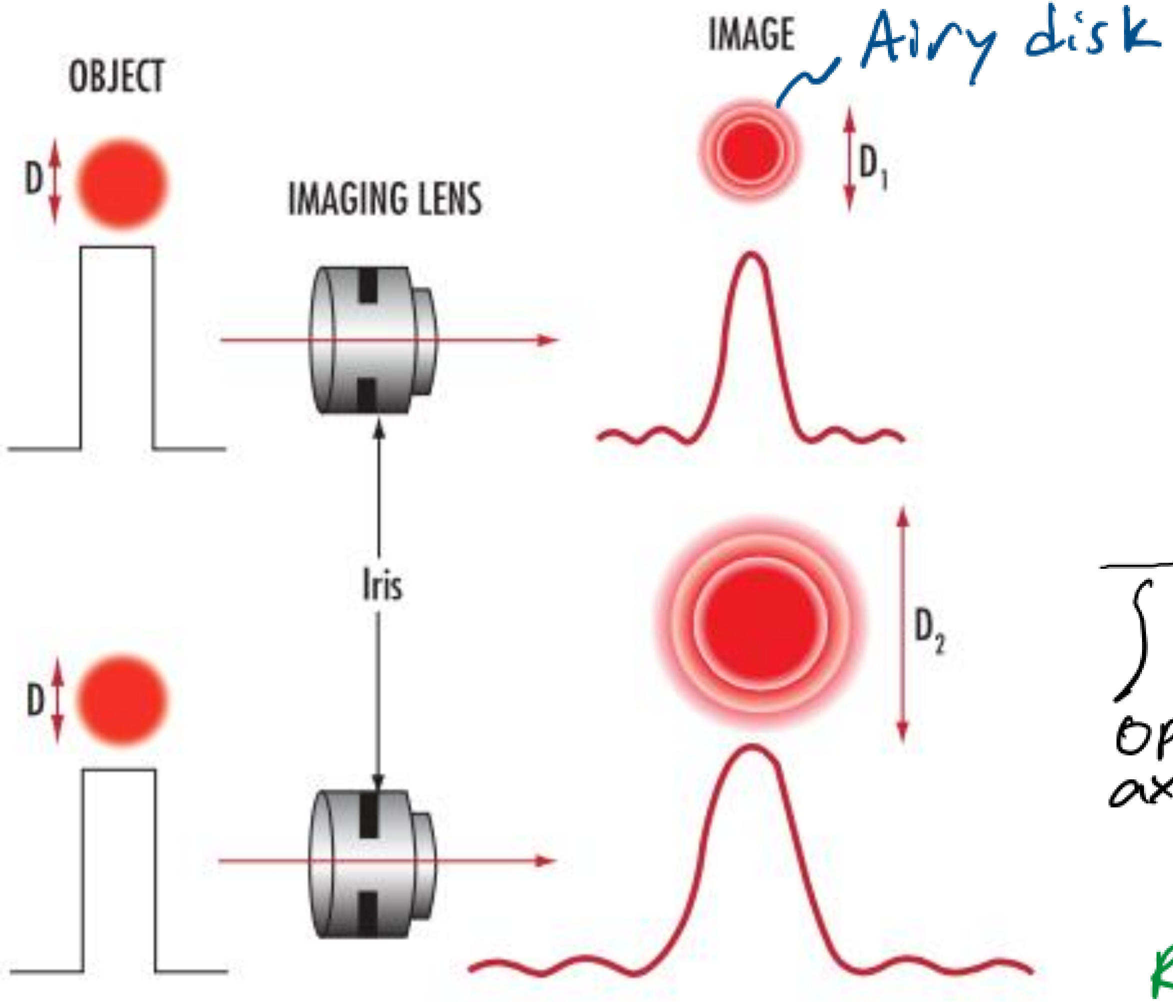
Microscopy of pollen grains

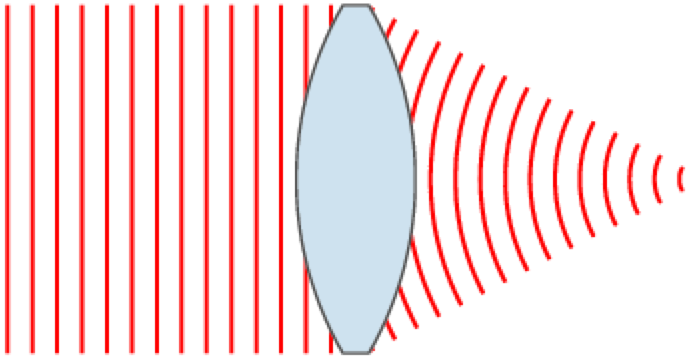


J. Li, PLOS ONE, Vol 8, e68957 (2013)

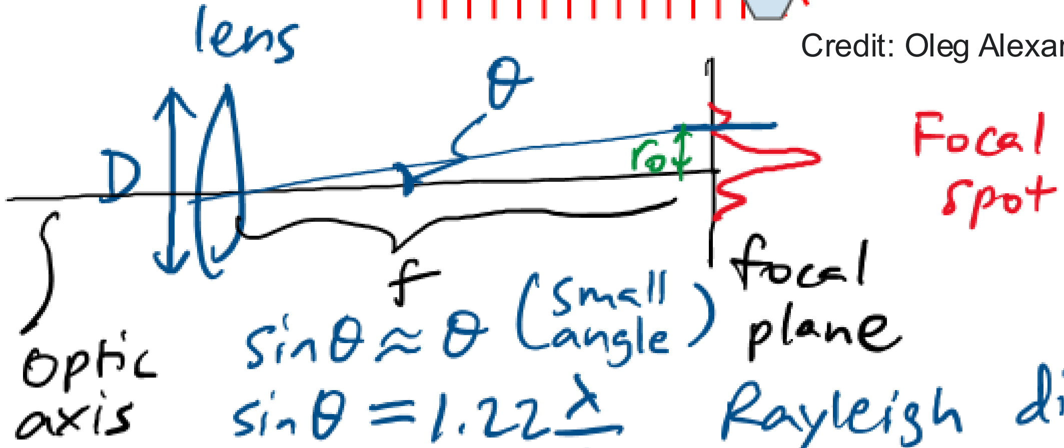
Diffraction limit in microscopy

- Diffraction arises from light or electron passing through optics (for example, a lens) with finite aperture sizes
  - Diffraction depends on the geometry of the aperture (circular pattern → Airy pattern)





Credit: Oleg Alexandrov



$\sin\theta \approx \theta$ (small angle)

$\sin\theta = 1.22\frac{\lambda}{D}$ Rayleigh diffraction

$r_0 = f\tan\theta \approx f\cdot\theta = 1.22\frac{f\lambda}{D}$

Resolution: $\Delta x = 2r_0 = 2.44 f\lambda/D$

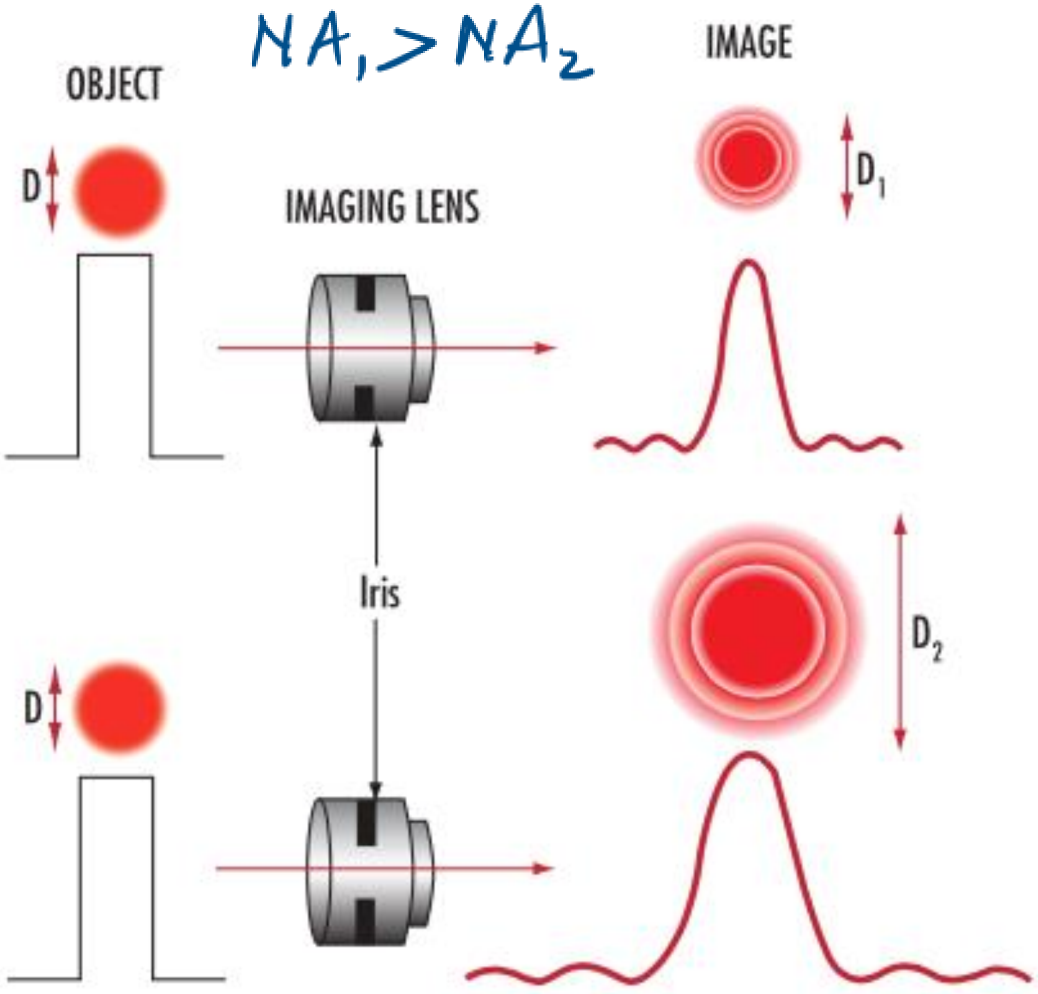
Diffraction limit in microscopy

- Diffraction arises from light or electron passing through optics (for example, a lens) with finite aperture sizes
  - Diffraction depends on the geometry of the aperture (circular pattern → Airy pattern)

$NA_1 > NA_2$

#1

#2

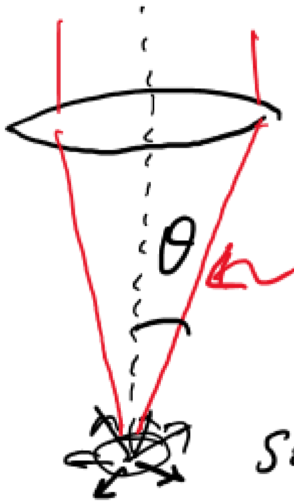


Numerical aperture

$NA \equiv n \sin\theta$

refractive index of medium

collection angle



lens

collection cone

light source

Diffraction limit:

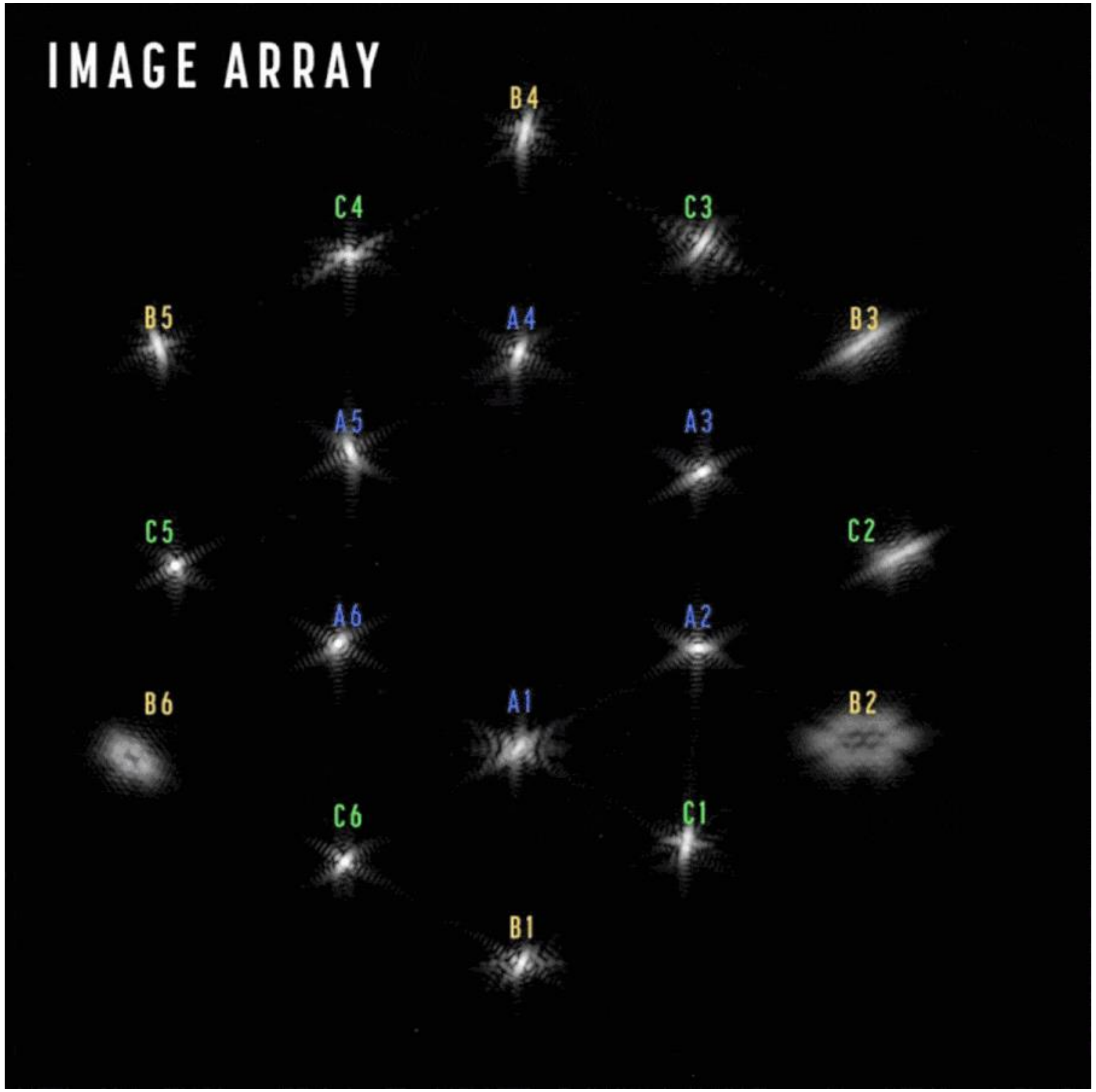
Rayleigh limit

$$\Delta x = \frac{1.22\lambda}{2NA}$$

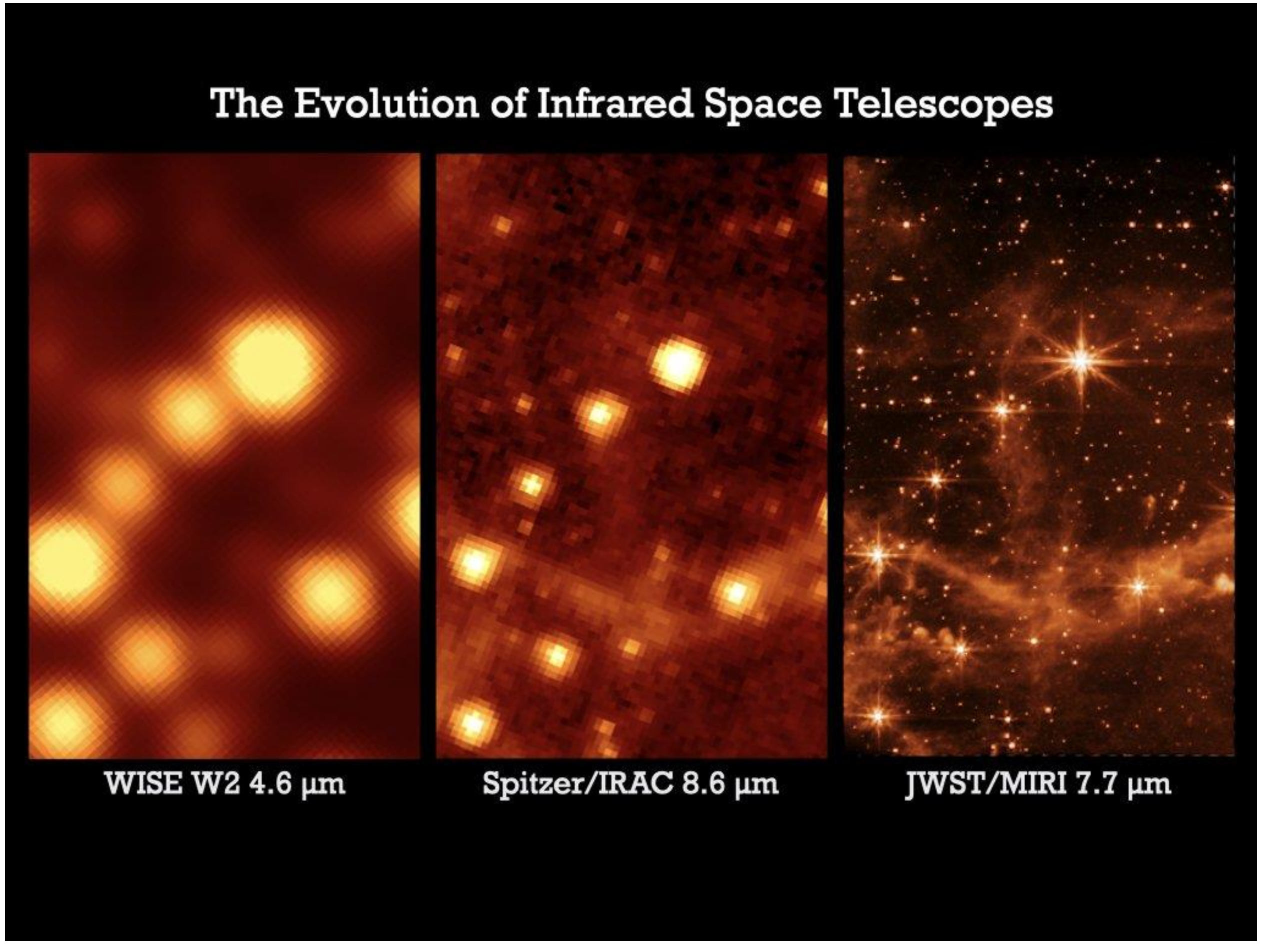
Abbe limit

$$\Delta x = \frac{\lambda}{2NA}$$

Highest resolution infrared image from space from the Webb Telescope



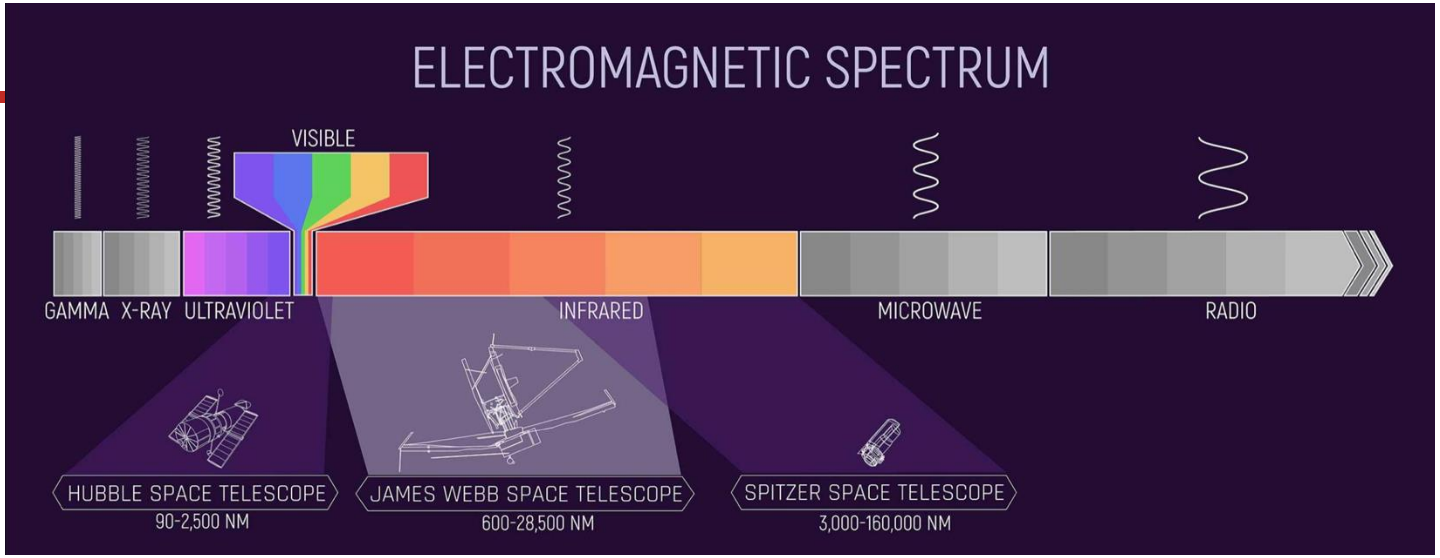
Star 2MASS J17554042+6551277



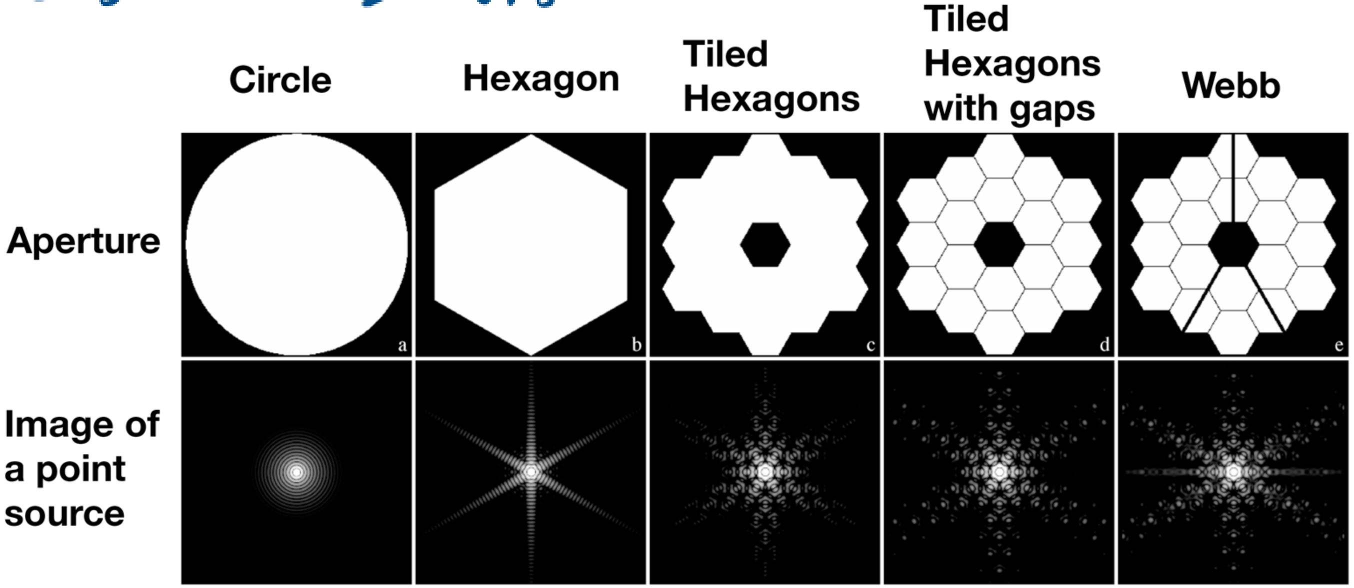
Credit: NASA/STScI

Optics of Webb Telescope

Infrared imaging + high angular resolution



D~2.5m D~6.5m



https://www.stsci.edu/files/live/sites/www/files/home/jwst/documentation/technical-documents/_documents/JWST-STScI-001157.pdf

Diffraction limit numerical examples

You are trying to study the structures of a cell using a light microscope and an electron microscope.

- The light microscope has a numerical aperture of 1.3 and uses green light with a wavelength of 550 nm. What is the diffraction limit of the microscope according to the Abbe limit?

$$\Delta x = \frac{\lambda}{2NA} = 211.5 \text{ nm}$$

- If the resolution of the image needs be improved by 1000 times with an electron microscope (whose numerical aperture is assumed to be 1), what is the accelerating voltage needed for the electron beam?

$$\lambda_e = \frac{211.5 \text{ nm}}{1000} \times 2 = .4 \text{ nm} \quad \text{or} \quad 4 \text{ Å}$$

Assume non-relativistic electrons $E_{kin} \ll m_e c^2 = 0.511 \text{ MeV}$

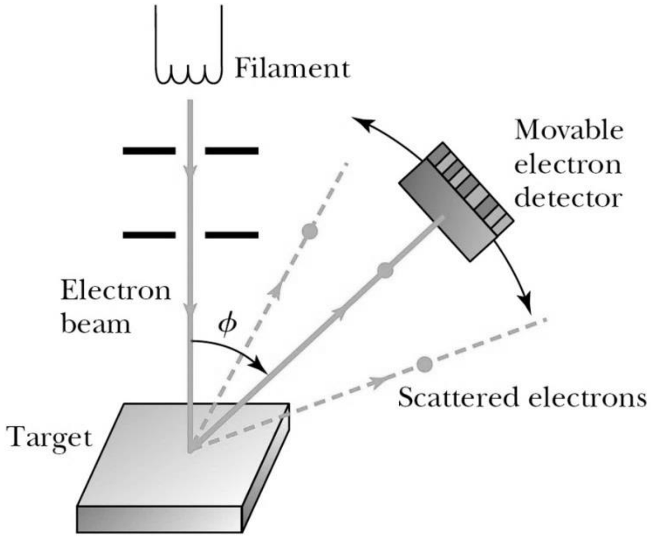
$$\lambda_e = \frac{hc}{\sqrt{2 E_{kin} m_e c^2}} \qquad E_{kin} = e \cdot V_a$$

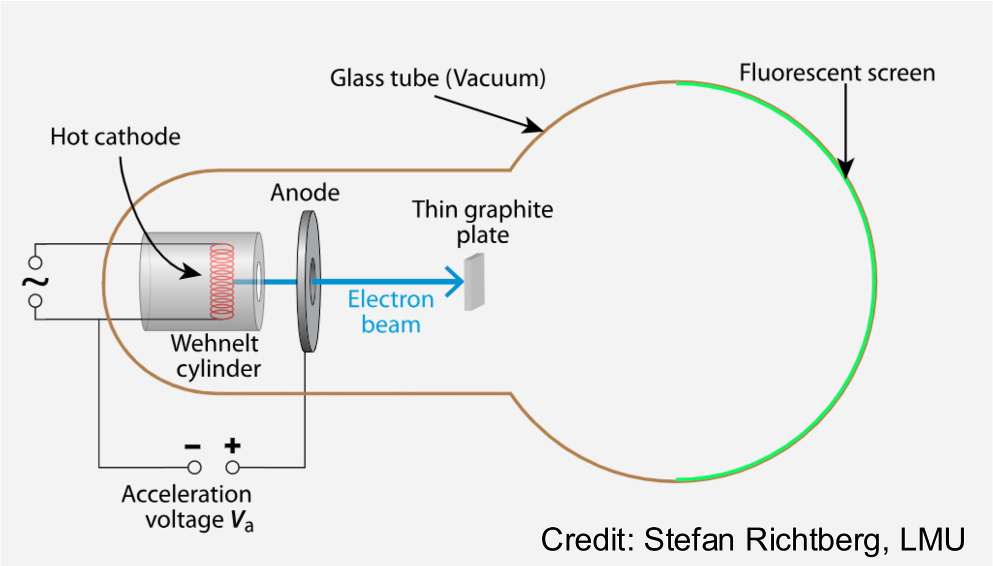
$$V_a \sim 8 \text{ V}$$

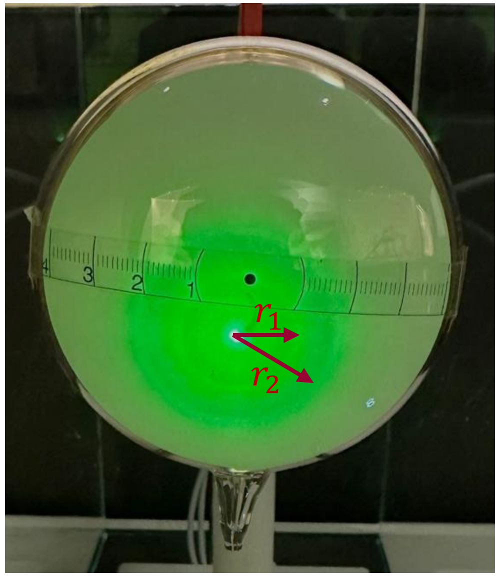
This acceleration voltage is much smaller than the ~ few to tens of keV typically used for electron microscopy. Experimentally, the distribution of electron energies will be narrower at these high energies. Additionally, electron beams are focused using electromagnetic lenses, which can cause aberrations such that the resolution is ultimately limited by the electron optics rather than the de Broglie wavelength.

How electron diffraction can be used to study crystal structure of materials

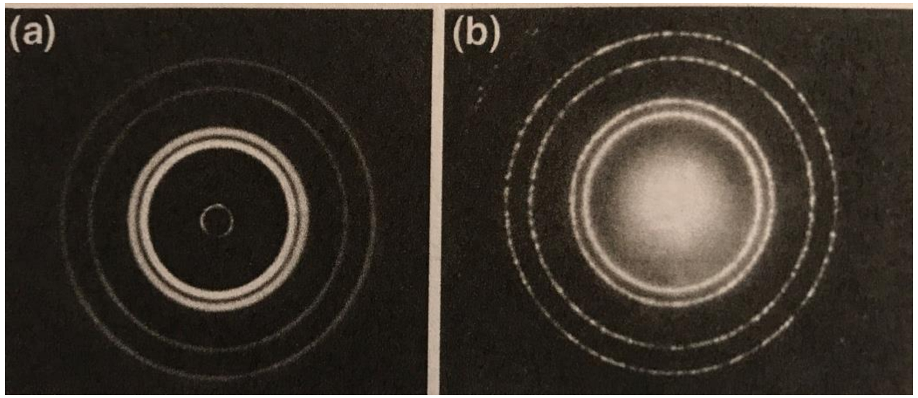
Electron diffraction







Diffraction of crystalline aluminum



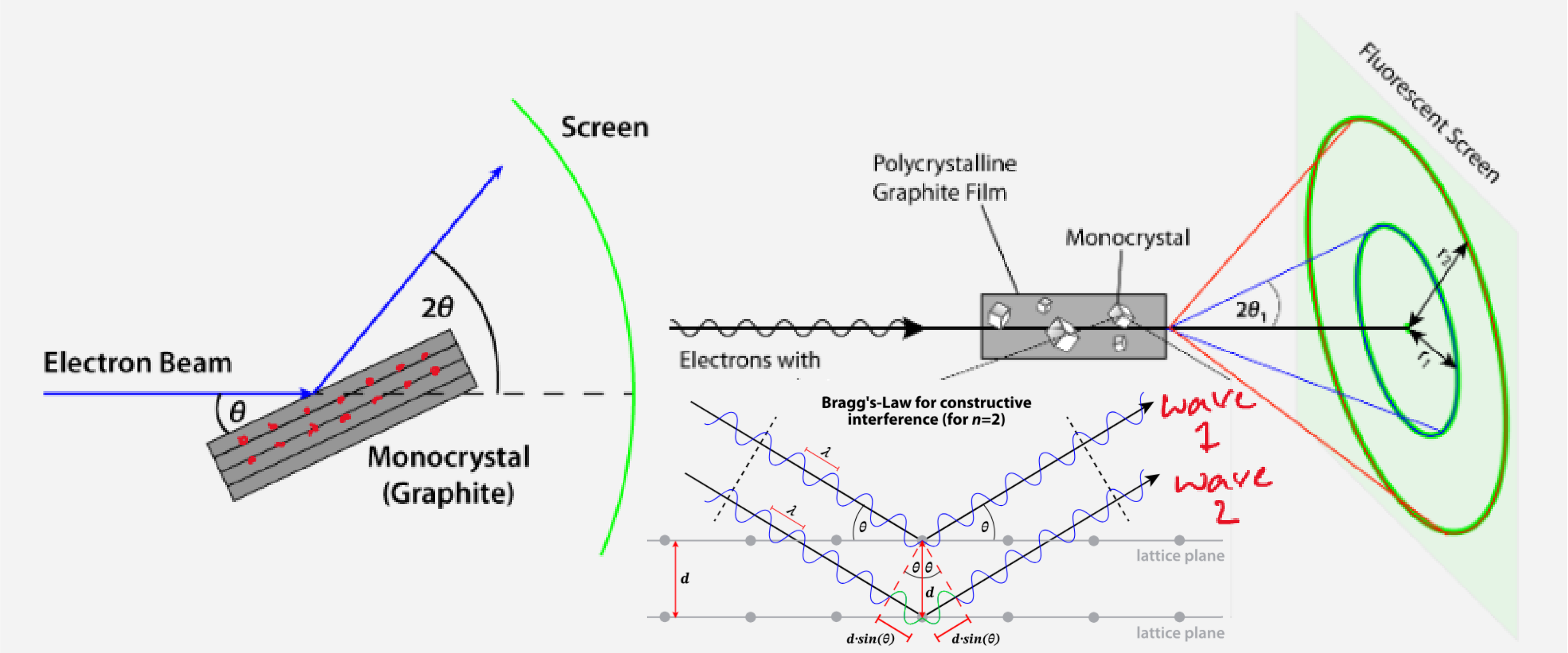
Electron X-ray

Top Hat question: as the acceleration voltage is increased, what happens to r_1 and r_2?

get smaller

Bragg diffraction with electrons

Why is the pattern circular? Polycrystallinity of sample



Pathlength difference between waves 1 & 2: $2d\sin\theta$

Constructive interference:

$$n\lambda = 2d\sin\theta$$

lattice spacing

integer #

de Broglie λ

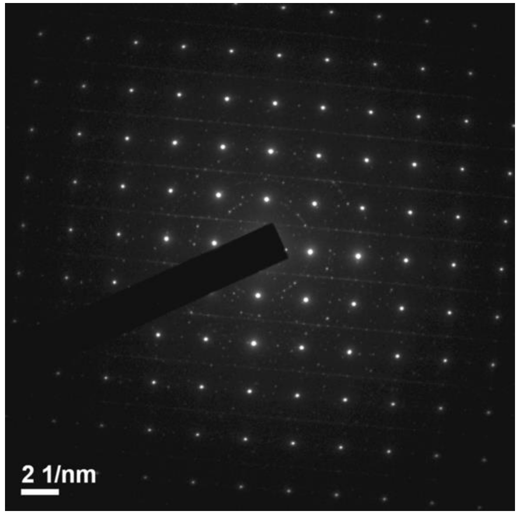
diffraction angle

https://virtuelle-experimente.de/en/elektronenbeugung/einfuehrung/bragg-bedingung.php

Electron diffraction problem

In an electron diffraction experiment, electrons are accelerated through a potential difference V to strike a thin <u>monocrystalline</u> silicon target. The first-order diffraction maximum is observed at an angle of $\theta = 50°$ from the direction of incoming electrons (the forward direction).

- Draw the diffraction pattern.



- If the accelerating voltage is 1500 V, what is the spacing d between the atomic layer of the crystal?

$$m\lambda = 2d\sin\theta$$

$$d \sim 0.2\,\text{Å}$$

$m = 1$

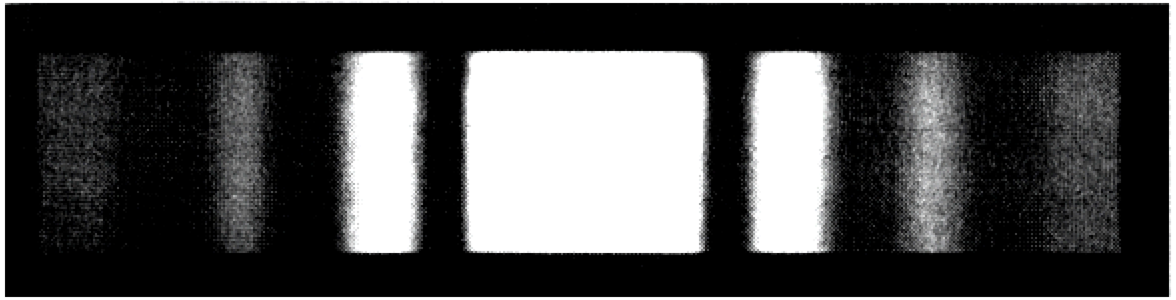
first-order diffraction

$$\lambda = \frac{hc}{\sqrt{2E_{kin}m_ec^2}}$$

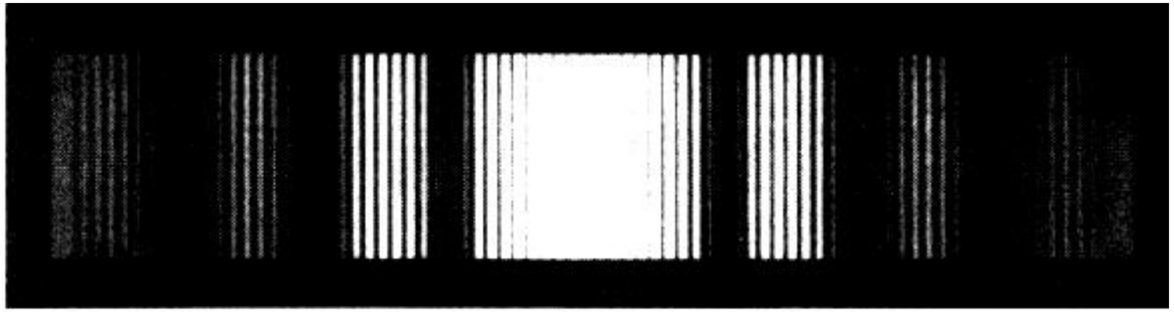
non-relativistic approx.

Fraunhofer diffraction patterns

One slit



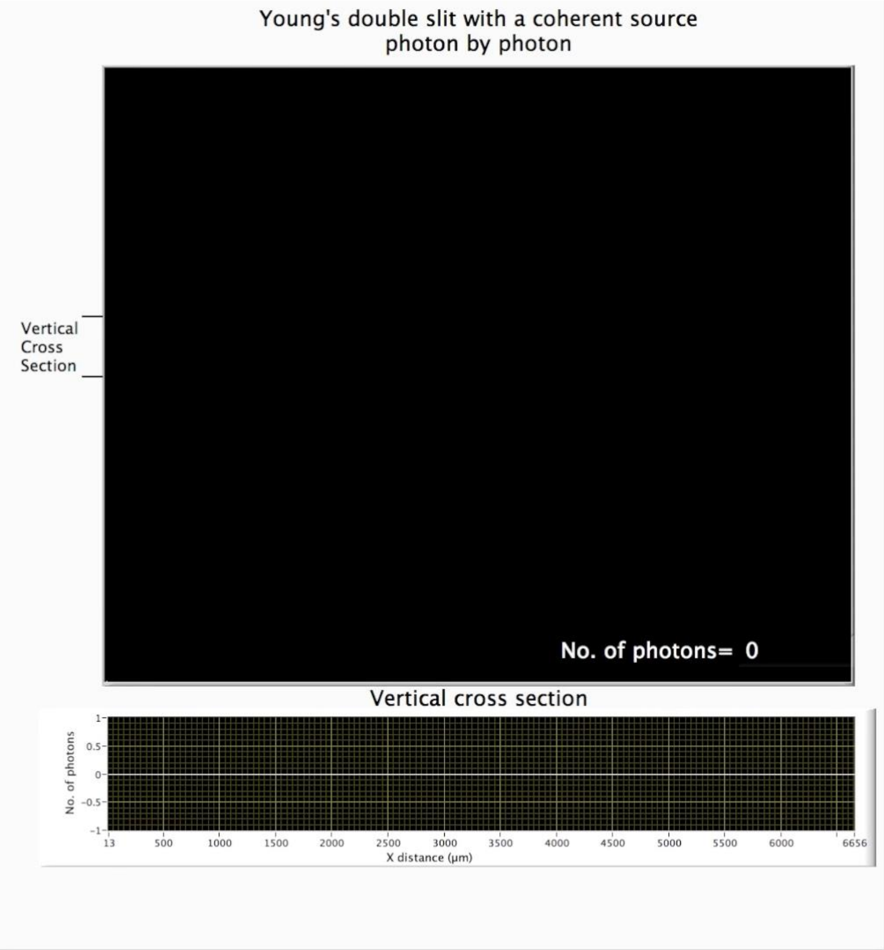
Two slits



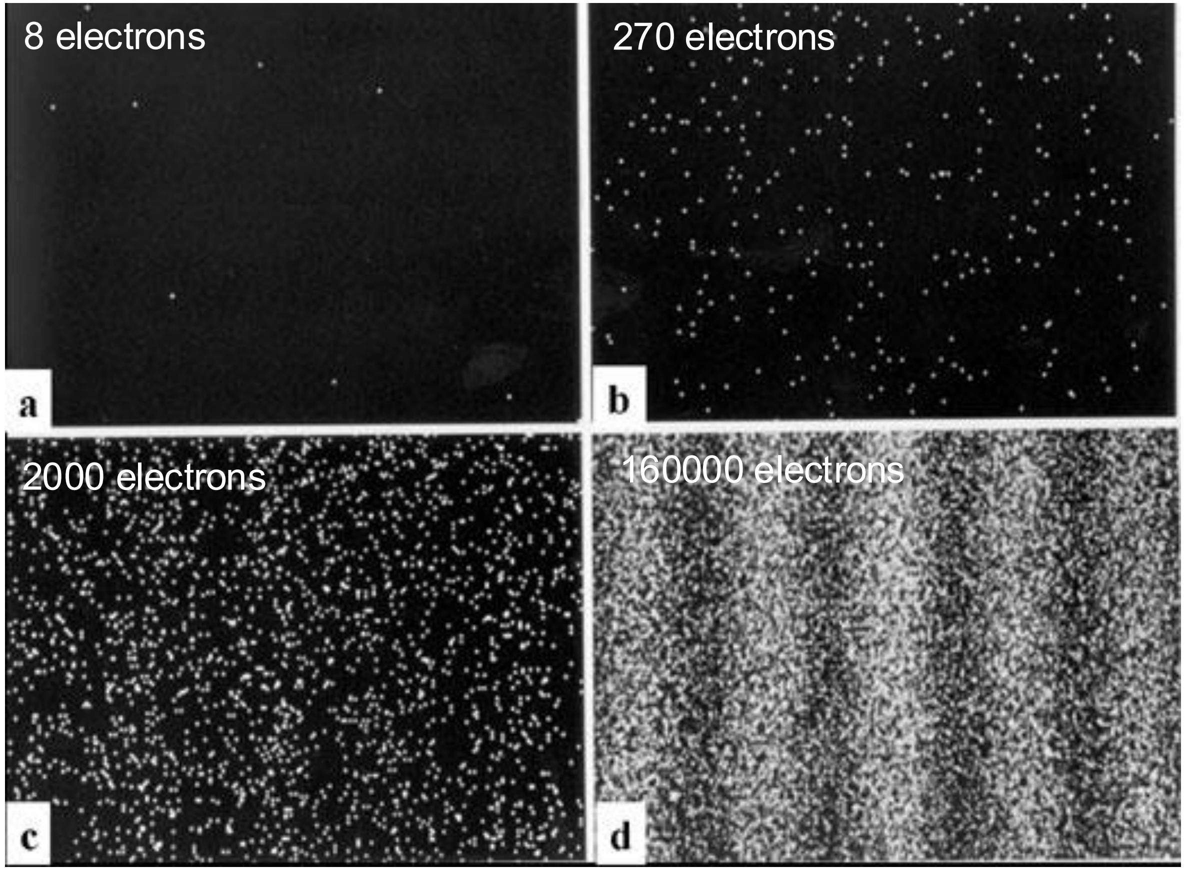
What happens when you send one photon or electron at a time?

Double-slit experiment in the single-particle limit

One photon at a time



One electron at a time



Still get double-slit diffraction pattern

R. Aspden and M. J. Padgett, American Journal of Physics 84 (2016)

Experiment by Tonomura et. al (1989)
https://www.hitachi.com/rd/research/materials/quantum/doubleslit/index.html

Wave functions of sub-atomic particles and atoms

- Define a wave function $\psi(x)$ that will determine the likelihood (or probability distribution density) $P(x)$ of finding a particle around a particular position in space:

$$P(x) \equiv |\psi(x)|^2$$

- The probability of the particle being between x_1 and x_2 is given by: $\int_{x_1}^{x_2} |\psi(x)|^2 \, dx$

- The total probability of finding the particle somewhere is 1.
  - Forcing this condition on the wave function is called normalization:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$

Slide from R. Trebino's lecture notes on Modern Physics

How to write a wave function

- Describe a particle with mass m and momentum p_0

EM waves

$$\mathcal{E} \propto \mathcal{E}_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)} \rightarrow \mathcal{E}_0 e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-Et)}$$

$$\vec{p} = \hbar\vec{k}$$

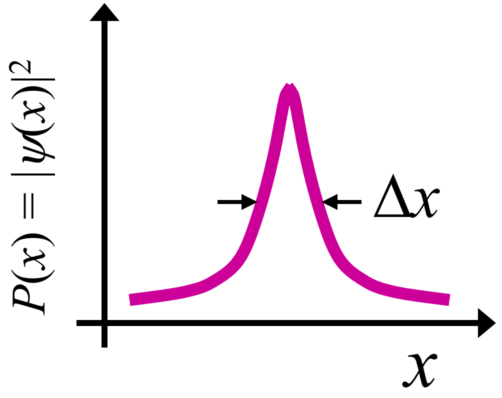
$$E = \hbar\omega$$

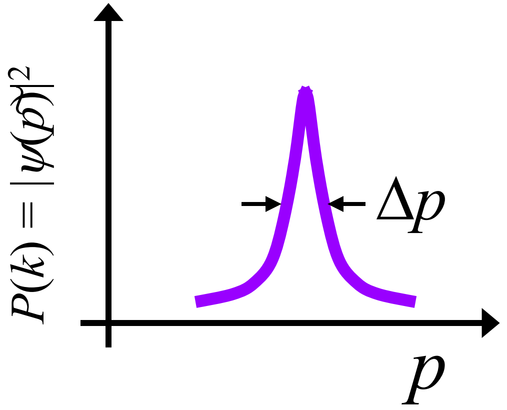
Assume particle in 1D:

$$\boxed{\Psi(x,t) \propto e^{\frac{i}{\hbar}(p_0 x - Et)} \; ; \; E = \frac{p_0^2}{2m}}$$

Probability distribution and uncertainty

- The probability distribution refers to the likelihood of measurement results of a quantity
  - **The width of the probability distribution is the uncertainty in the measurement of that quantity**
- We can analogously define probability distributions of other quantities that we might wish to measure.
- For example, we can Fourier transform $\psi(x)$ with respect to x and find $\psi(p)$.





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Heisenberg's uncertainty principle

- **For momentum and position**: $\Delta p \, \Delta x \geq \hbar/2$
  - Cannot simultaneously measure the precise values of p and x for a wave.
- **For energy and time:** $\Delta E \, \Delta t \geq \hbar/2$
  - Cannot simultaneously measure the precise values of t and E for a wave.
  - Measurements over a time Δt cannot determine the energy to better than $\Delta E \geq \hbar/(2\Delta t)$.
- Heisenberg's uncertainty relations $\Delta x \Delta p \geq \frac{\hbar}{2}$ and $\Delta \mathrm{E} \Delta t \geq \frac{\hbar}{2}$ place lower limits to the uncertainties in simultaneously determining position and momentum, and energy and time.
  - Can define similar relations for conjugate variables that are related by a Fourier transform

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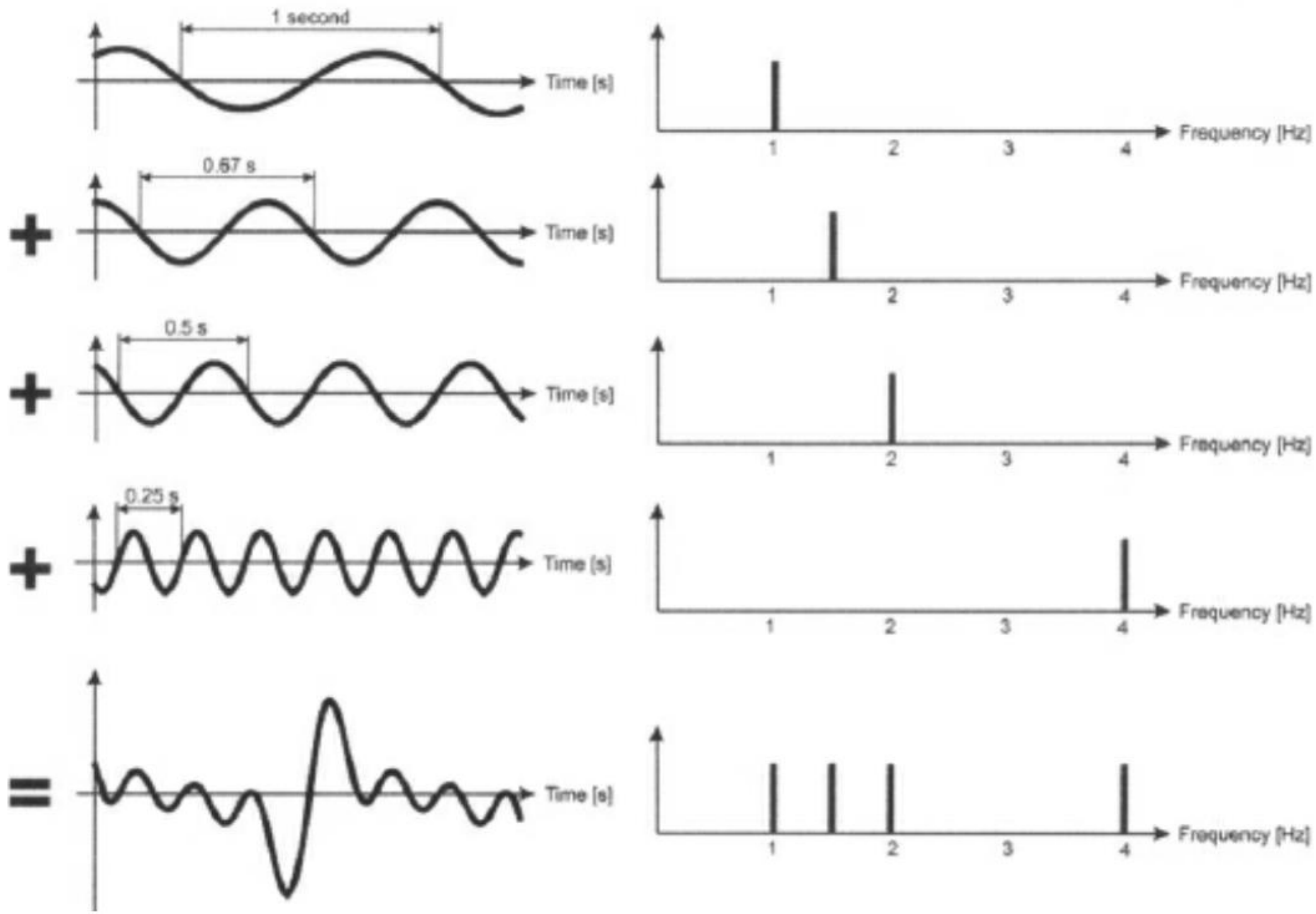
Analogy to Fourier analysis

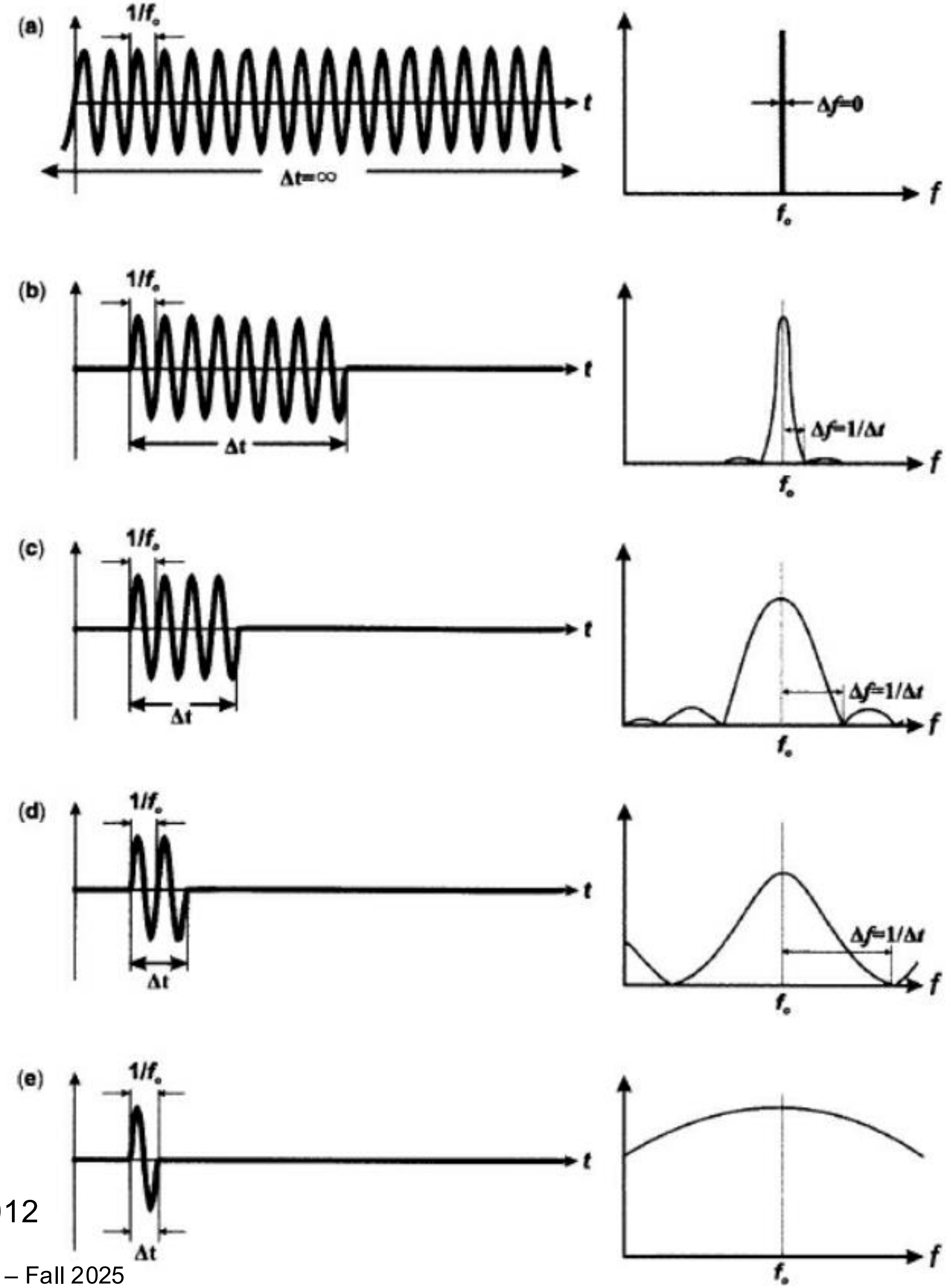
- Fourier analysis: a time-varying signal can be represented by frequencies of its sine wave components



D. Prutchi and S. R. Prutchi, Exploring Quantum Physics through Hands-on Projects, 2012

Analogy to Fourier analysis

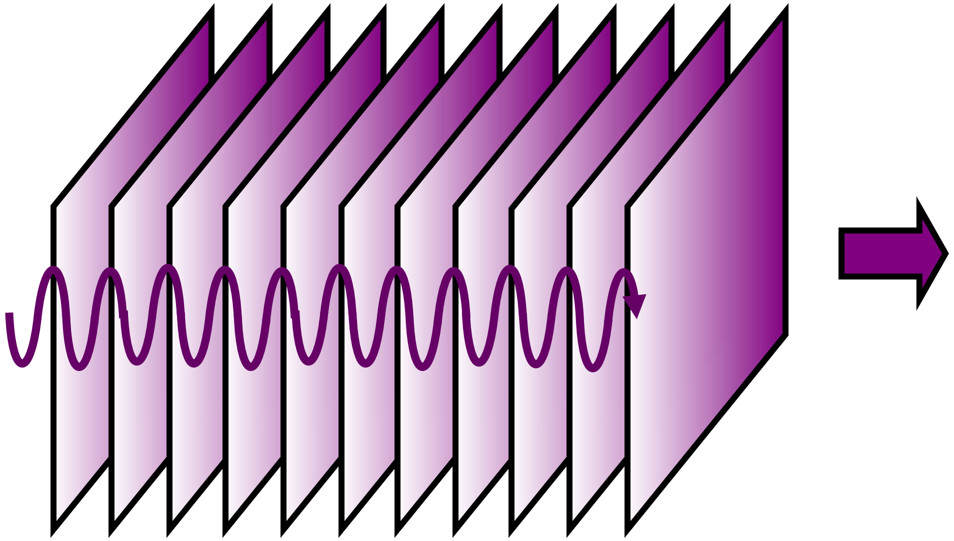
- Fourier analysis: a time-varying signal can be represented by frequencies of its sine wave component
- Width of the Fourier spectrum of a truncated sine signa depends on the measurement time
- Energy-time uncertainty:



D. Prutchi and S. R. Prutchi, Exploring Quantum Physics through Hands-on Projects, 2012

The uncertainty principle is derived from the wave nature of matter

- The plane-wave model we have been using for electromagnetic and matter waves is not physical: $\psi(x,t) \propto e^{i(kx-\omega t)}$ is associated with waves that are extended infinitely into the y and z directions, with wavefronts perpendicular to x.
    - Cannot be normalized
    - Fix this by defining a wave packet that localizes the matter wave within a spatial interval Δx

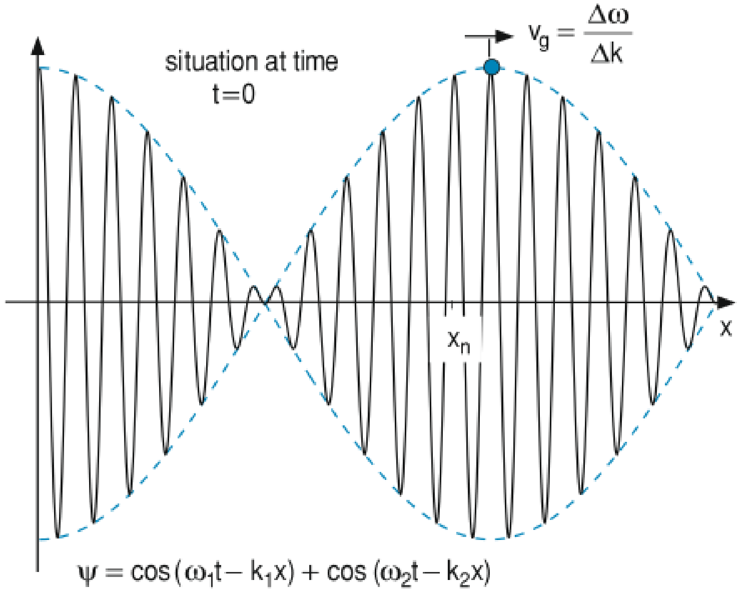


- A wave packet comprises of superposition of monochromatic waves with frequencies ω_j in interval $\Delta\omega$

$$\psi(x,t) = \sum_j c_j e^{i(k_j x - \omega_j t)}$$

- Extend superposition to include an infinite number of waves in which $\omega_0 - \frac{\Delta\omega}{2} \leq \omega \leq \omega_0 + \frac{\Delta\omega}{2}$ and $k - \frac{\Delta k}{2} \leq k \leq k_0 + \frac{\Delta k}{2}$:

$$\psi(x,t) = \int_{k_0-\frac{\Delta k}{2}}^{k_0+\frac{\Delta k}{2}} C(k) e^{i(kx-\omega t)} dk$$



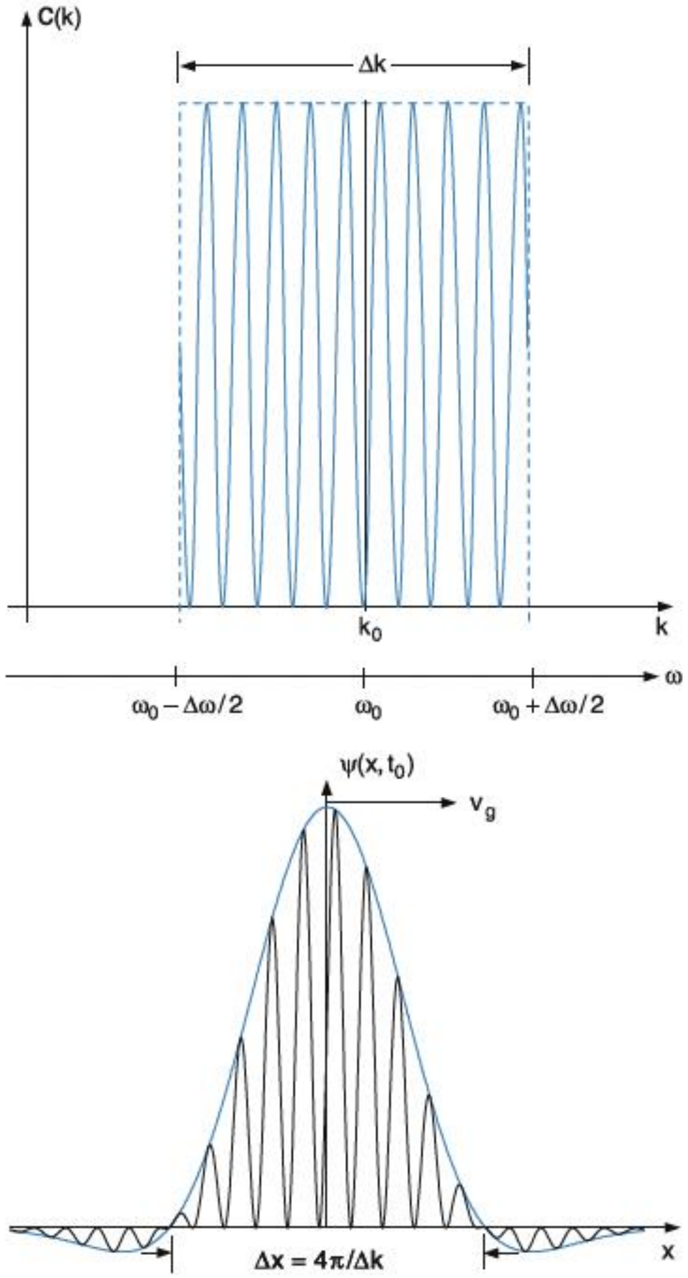
Wave packets

$$\psi(x,t) = \int_{k_0-\frac{\Delta k}{2}}^{k_0+\frac{\Delta k}{2}} C(k) e^{i(kx-\omega t)} dk$$

One possible solution:

$$\psi(x,t) = A(x,k,t) e^{i(k_0 x - \omega_0 t)}$$

$$A(x,k,t) = \frac{2C(k_0)\sin\left(\frac{u\Delta k}{2}\right)}{u}, \text{ where } u = \left(\frac{d\omega}{dk}\right)_{k_0} t - x$$



Source: Demtroder, Chapter 3

Group velocity and width of a wave packet

- Group velocity equals particle velocity

$$v_{gr} = v_p$$

- Wave vector of group center determines particle momentum

$$\boldsymbol{p_p} = \hbar \boldsymbol{k_0}$$

- At time t = 0, the width of the wave packet has a minimum value equal to the de Broglie wavelength

$$\Delta x(t=0) = \frac{4\pi}{\Delta k} \geq \lambda_{de\ Broglie}$$
$$\Delta x(t) \geq \lambda_{de\ Broglie}$$

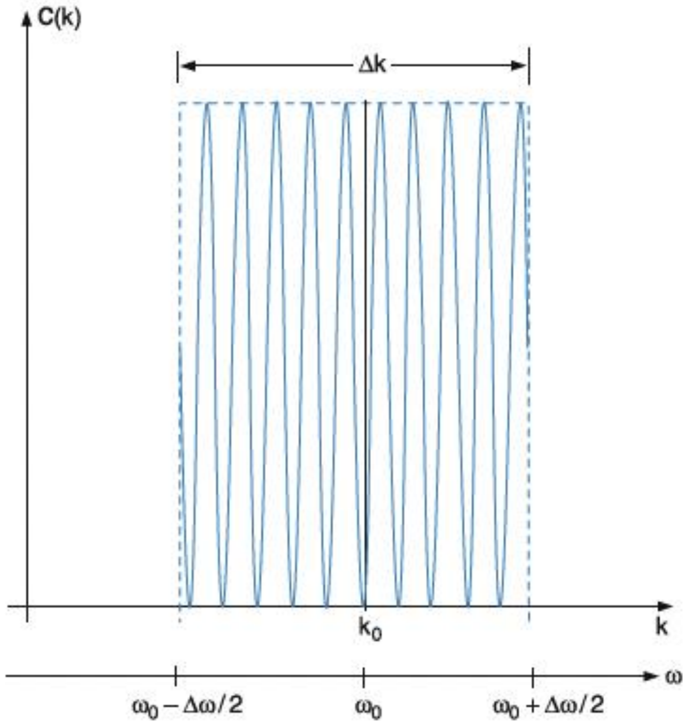
- How quickly the wave packet spreads in space depends on its initial momentum uncertainty:

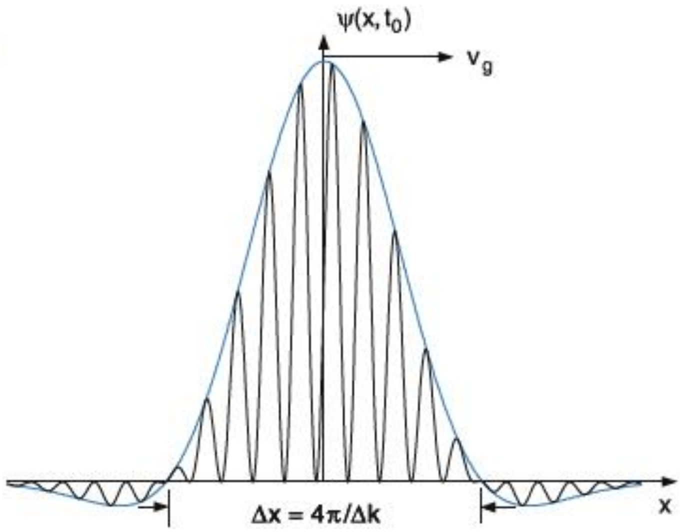
$$\frac{d\Delta x}{dt} \propto \frac{\Delta p(t=0)}{m}$$

Given two wavepackets with:

a : $\Delta k(t=0) = k_0$; **b :** $\Delta k(t=0) = 10\ k_0$

- Which will have a larger Δx at time $t = 0$?
- Which will have a faster increase in Δx?

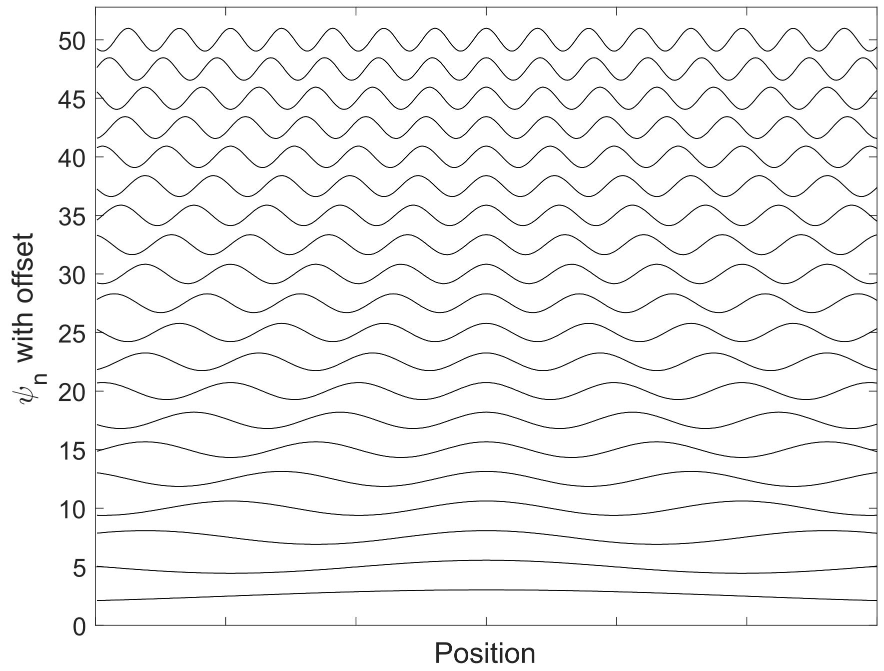


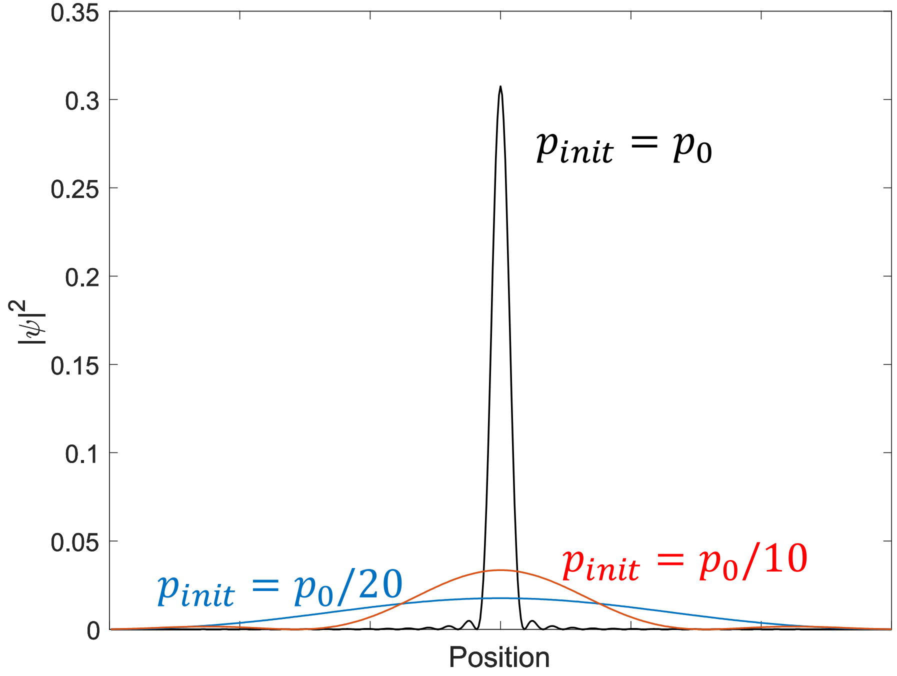


Source: Demtroder, Chapter 3

Visualizing wave packets: effect of initial momentum

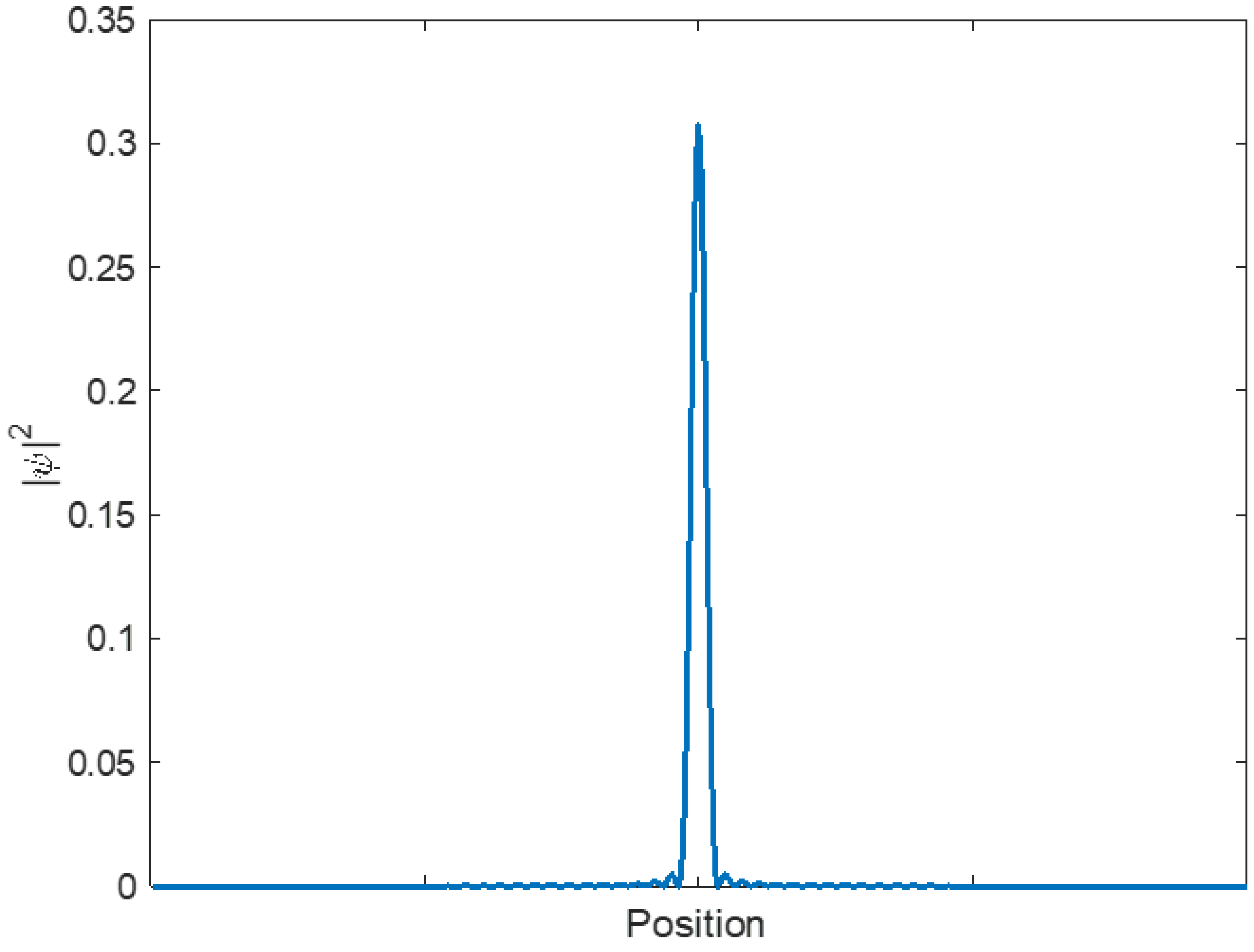
$\psi(x,t) = \sum_j c_j e^{i(k_j x - \omega_j t)}$, with initial momentum p_{init}



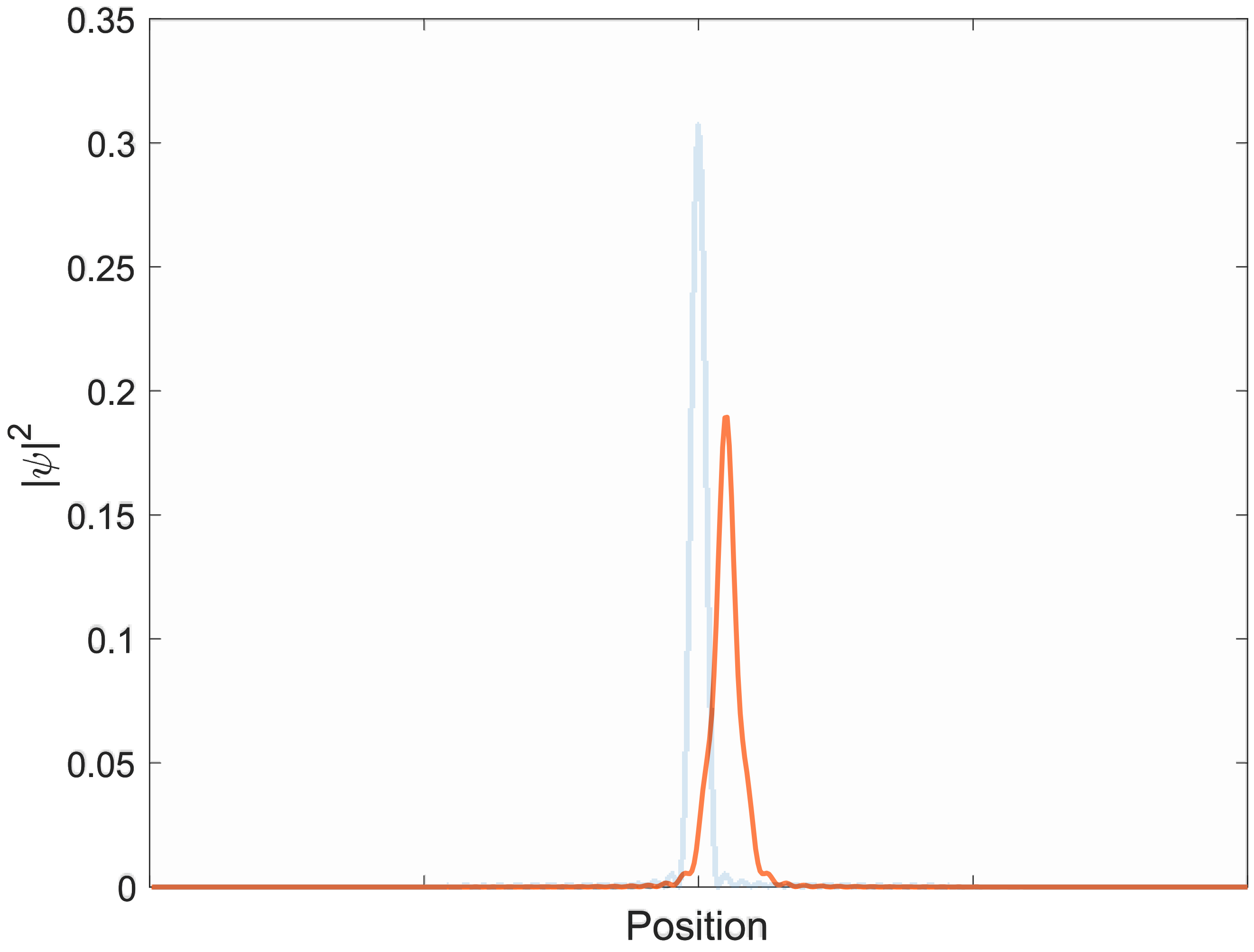


See MATLAB code wavepacket.m

Visualizing wave packets: change with increasing time



Visualizing wave packets: change with increasing time



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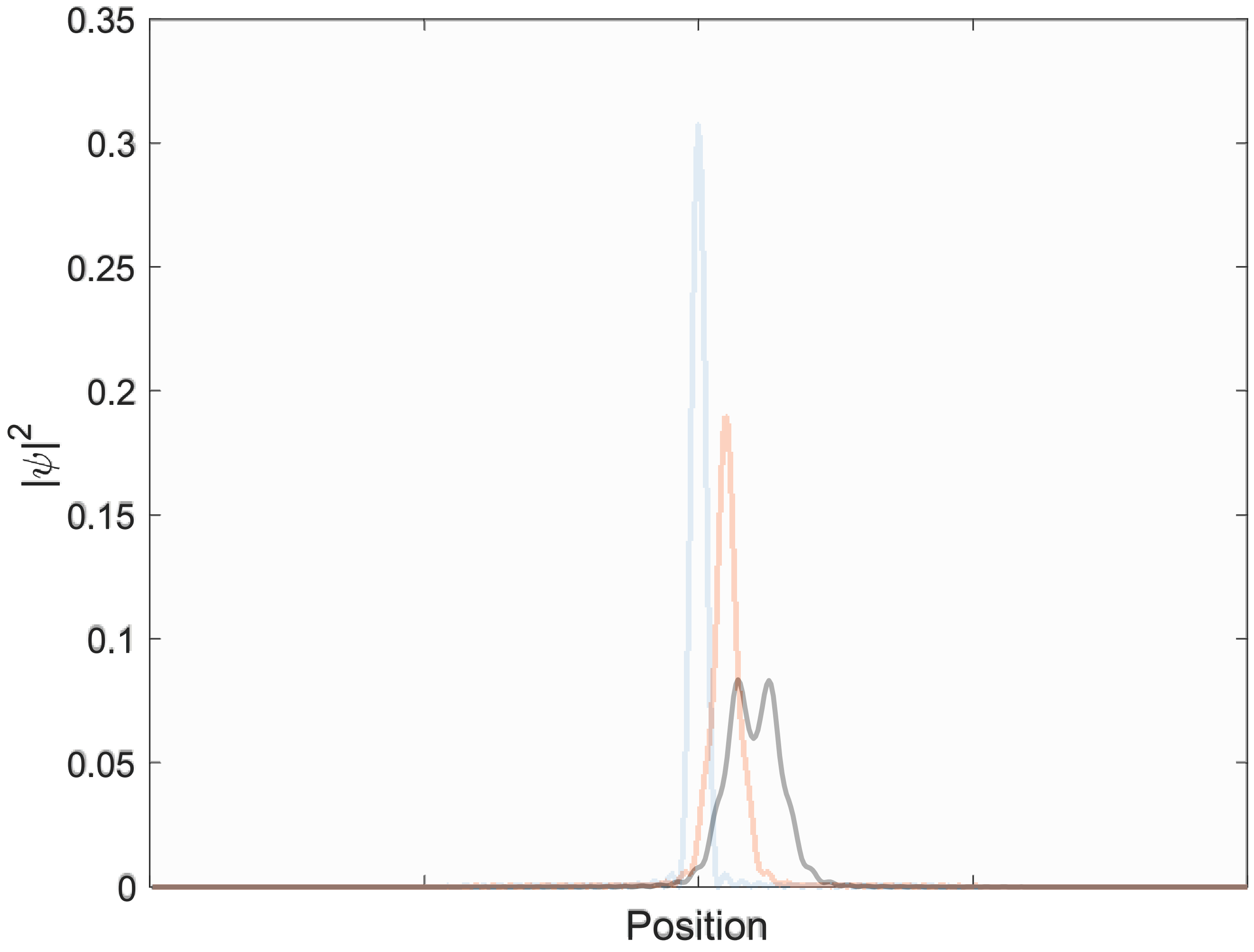

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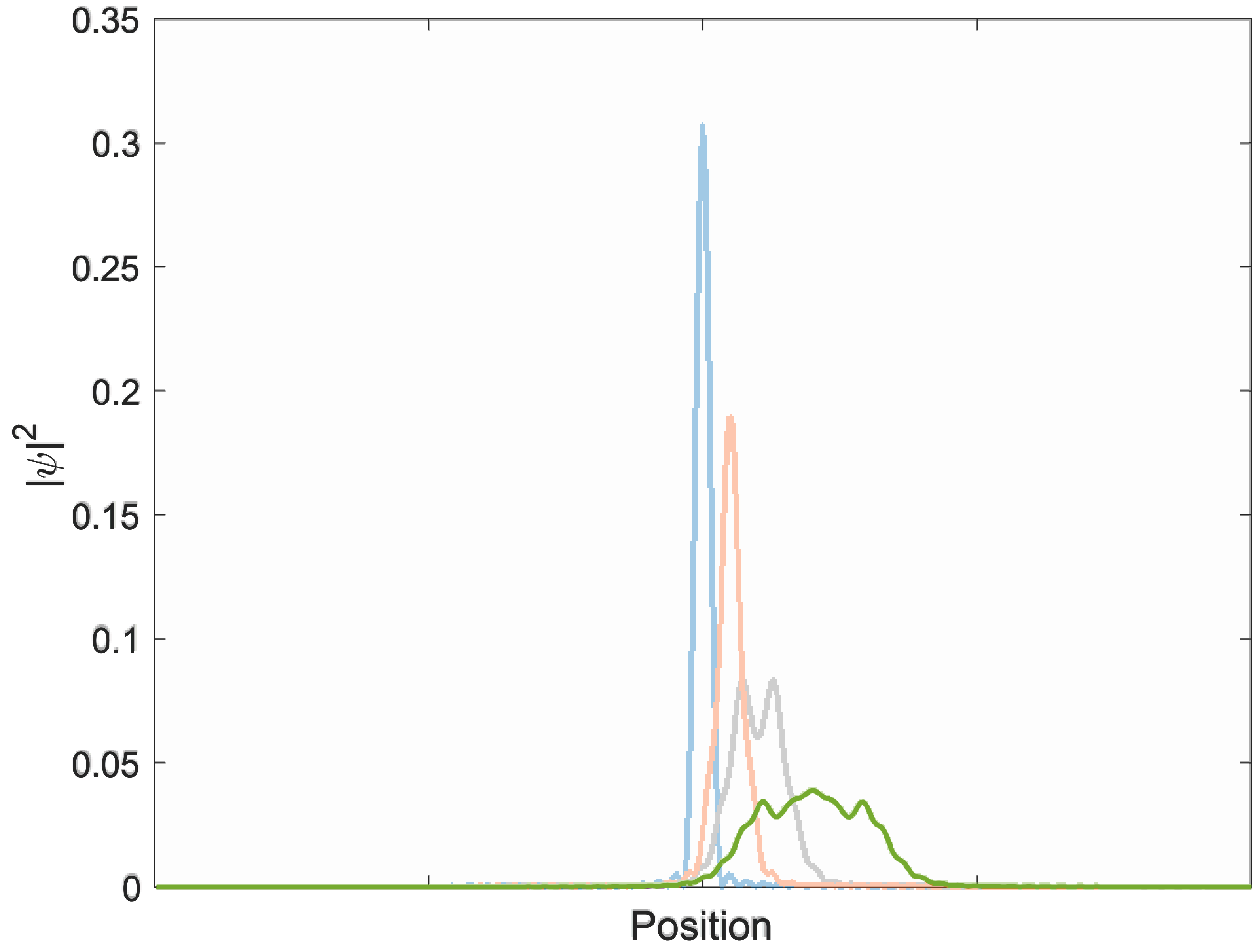
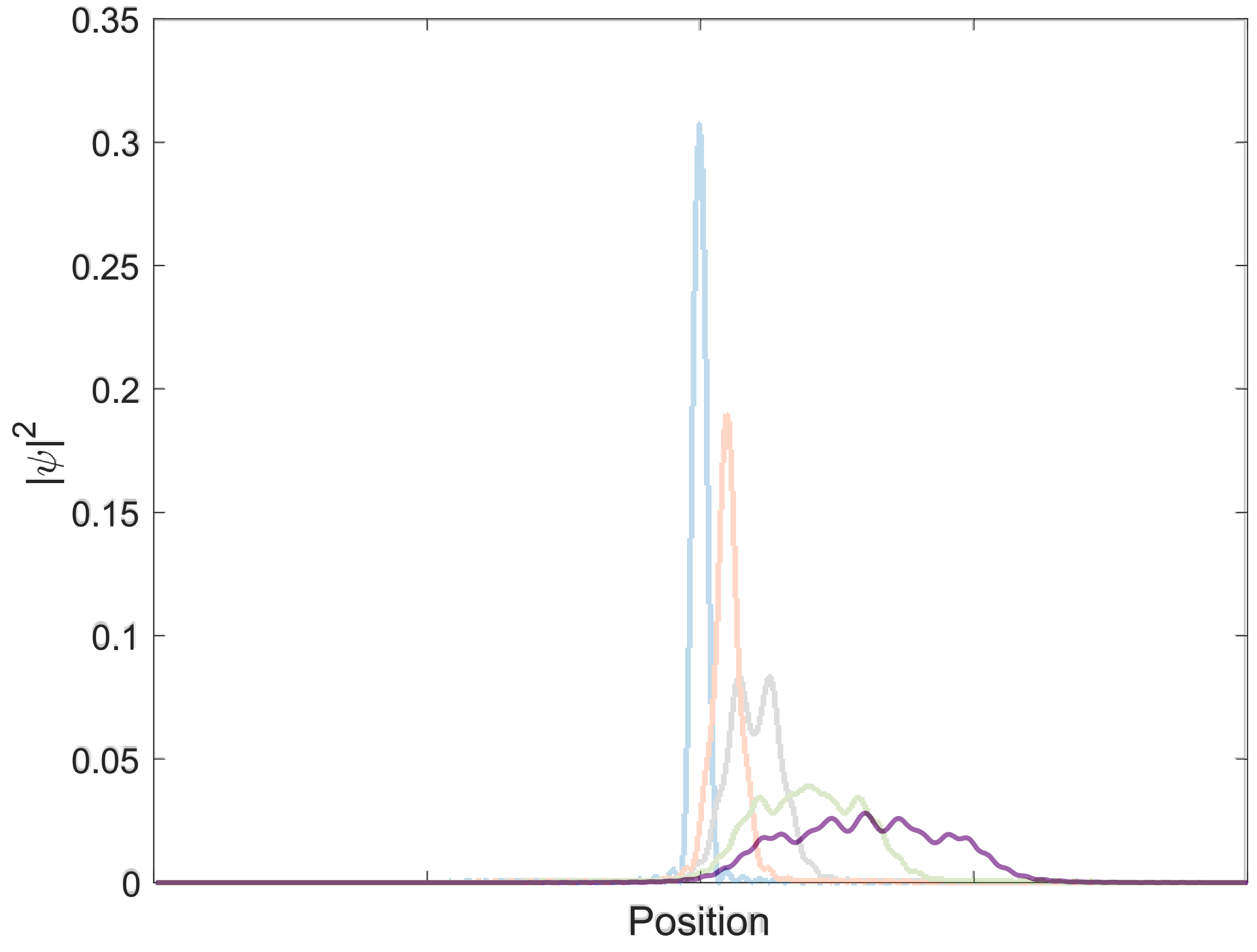
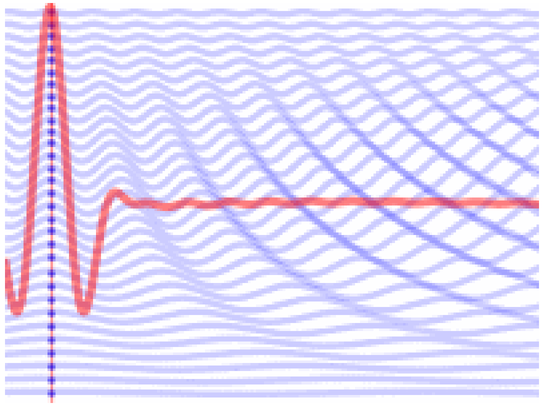


Visualizing wave packets: change with increasing time



Wave packet summary



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- Combination of plane wave solutions $\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}dk$
  - Carries a range of k values and therefore energy and momentum
  - Use initial conditions to find $\phi(k)$; *e.g.*, $\psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{ikx}dk$
  - Fourier transform: $\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x,0)e^{-ikx}dx$
- Group and phase velocities:
  - Group velocity is the dispersion $v_{\text{gr}} = \frac{d\omega}{dk} = \frac{\hbar k}{m} = v_p$, which corresponds to the classical particle velocity
    - It describes how fast the envelope of the wave packet is moving
  - Phase velocity $\frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{v_{gr}}{2}$
    - It describes how fast the individual wave function components are moving (not much physical meaning here)
- Why $\phi(k)$ is often modeled with a Gaussian function: provides the minimum uncertainty at t = 0.

How fast of a measurement time do we need to measure an electron wave packet?

An electron is localized in a hydrogen atom and moving at an average speed of $v = 2.2 \times 10^{6}\ m/s$ in a region of size $\Delta x = 5 \times 10^{-11}\ m$. We are to use a light pulse to image the electron wave packet without significantly disturbing it. The rest mass of electron is $m_e = 9.109 \times 10^{-31}\ kg$.

- What is the momentum uncertainty of the electron wave packet? Answer on Canvas.
- Estimate the duration of the light pulse required to resolve the wave packet.

The Nobel Prize in Physics 2023

Ill. Niklas Elmehed © Nobel Prize Outreach

Pierre Agostini

Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach

Ferenc Krausz

Prize share: 1/3

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Anne L'Huillier

Prize share: 1/3

The Nobel Prize in Physics 2023 was awarded to Pierre Agostini, Ferenc Krausz and Anne L'Huillier "for experimental methods that generate attosecond pulses of light for the study of electron dynamics in matter"

Attosecond electron wave packet interferometry

T. REMETTER[1], P. JOHNSSON[1], J. MAURITSSON[2], K. VARJÚ[1], Y. NI[3], F. LÉPINE[3], E. GUSTAFSSON[1], M. KLING[3], J. KHAN[3], R. LÓPEZ-MARTENS[4], K. J. SCHAFER[2], M. J. J. VRAKKING[3] AND A. L'HUILLIER[1]*

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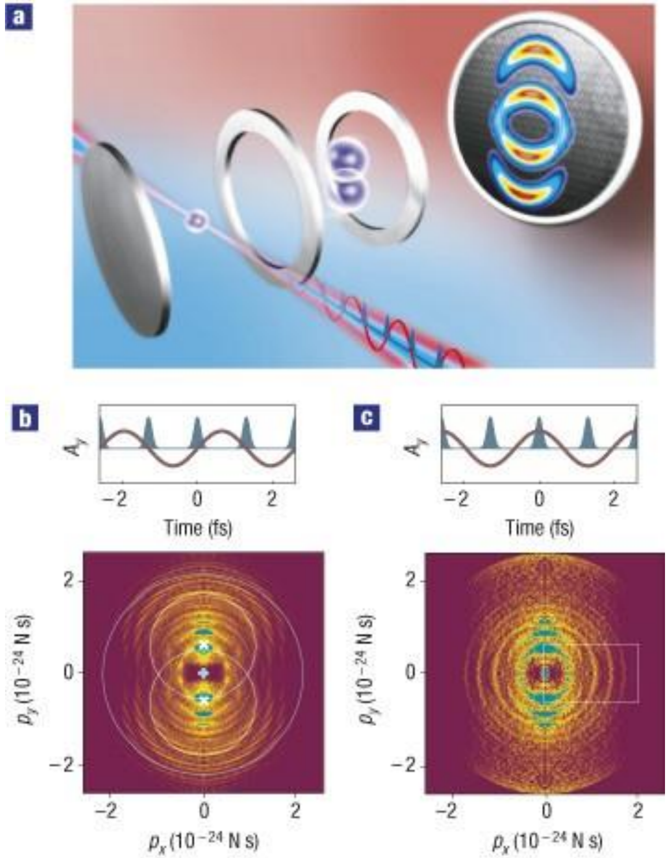

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