UNIVERSITÀ DEGLI STUDI DI TRIESTE

Scienza dei Materiali
-lecture 3-

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Quantum mechanics – basic concepts

1. Introduction of quanta: Plank (black body radiation), Einstein (Photoelectric Effect*)

2. Wave-particle dualism: Einstein (P.E. effect), De Broglie (Matter Waves*)

3. Matter waves and wavepackets

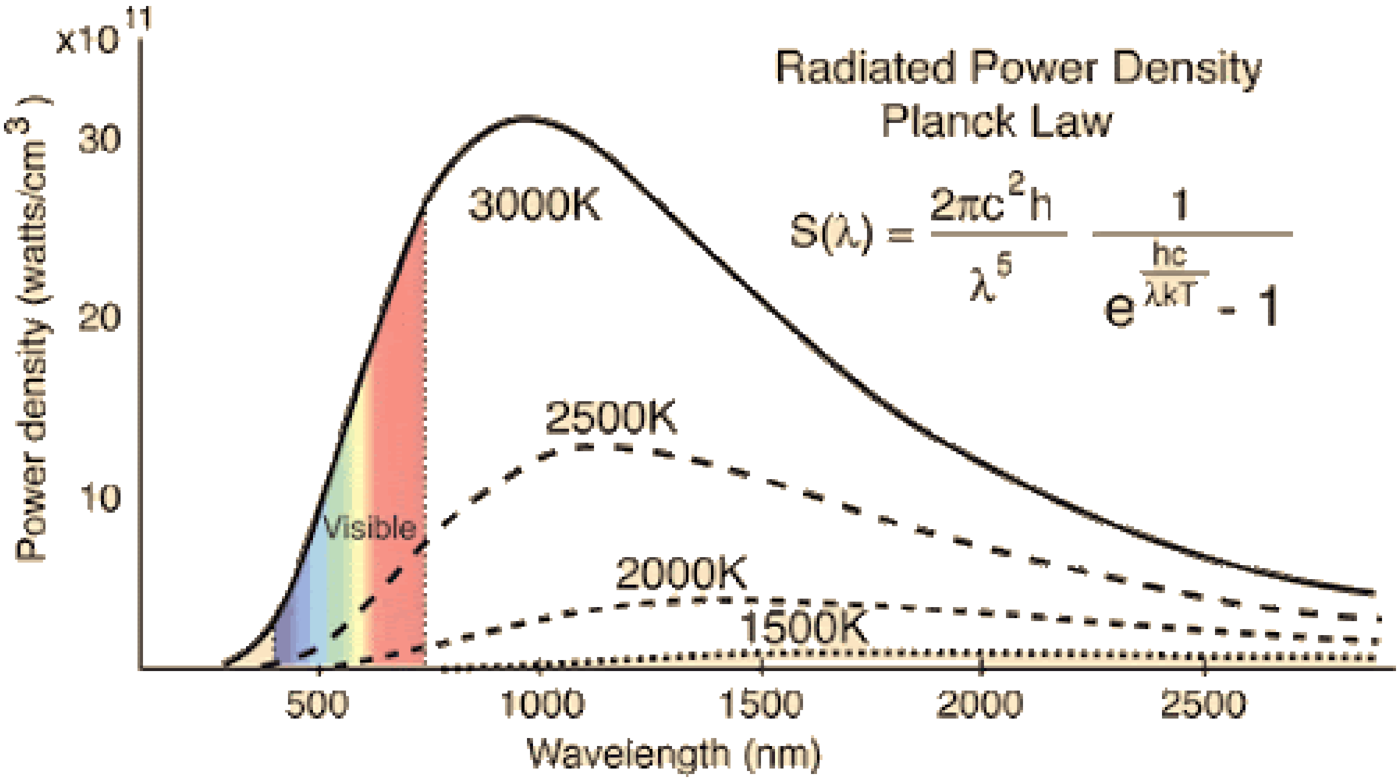
4. Uncertainty

5. Statistical approach

6. Waves and wave equation

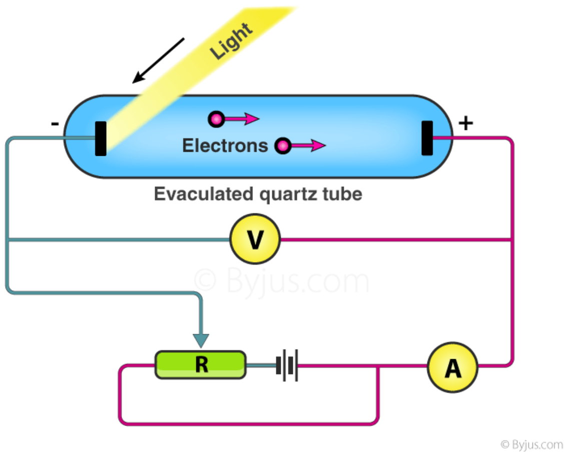
7. Schroedinger Equation

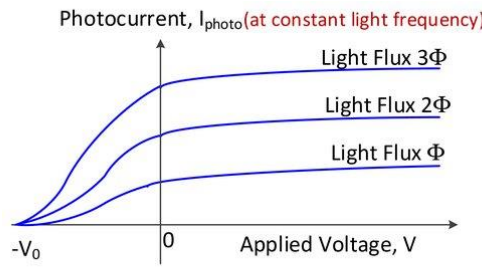
Quantum mechanics
Black body radiation

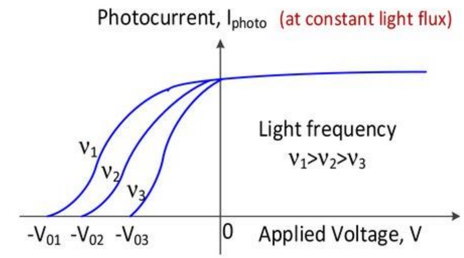


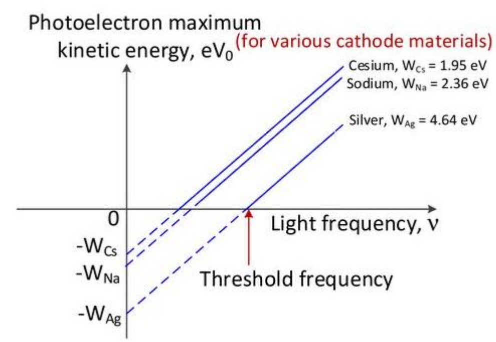
*Sidetrack: Photoelectric Effect

Hertz Experiments







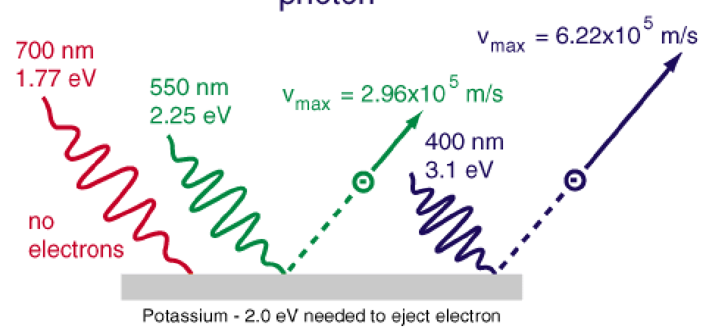


Einstein’s hypotheses for explaining the effect:

- Radiation is made up of photons
- Photons are absorbed or emitted in descrete amounts
- Photon energy is $\propto h\nu$
- Photons behave like waves

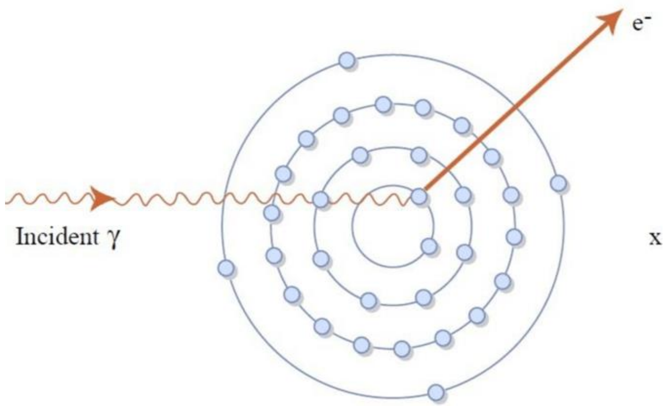
$$E_{kin} = h\nu - W$$

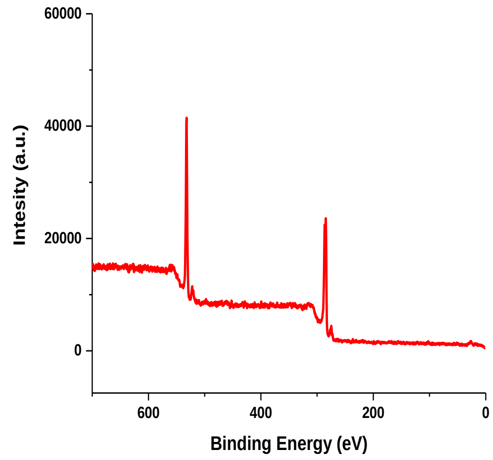
$$E_{photon} = h\nu$$

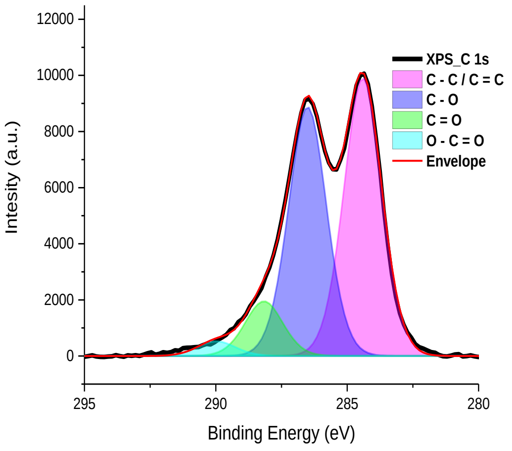


*A sidetrack: Photoelectric Effect

Application of the photoelectric effect: X-Ray Photoelectron Spectroscopy (XPS, ESCA)

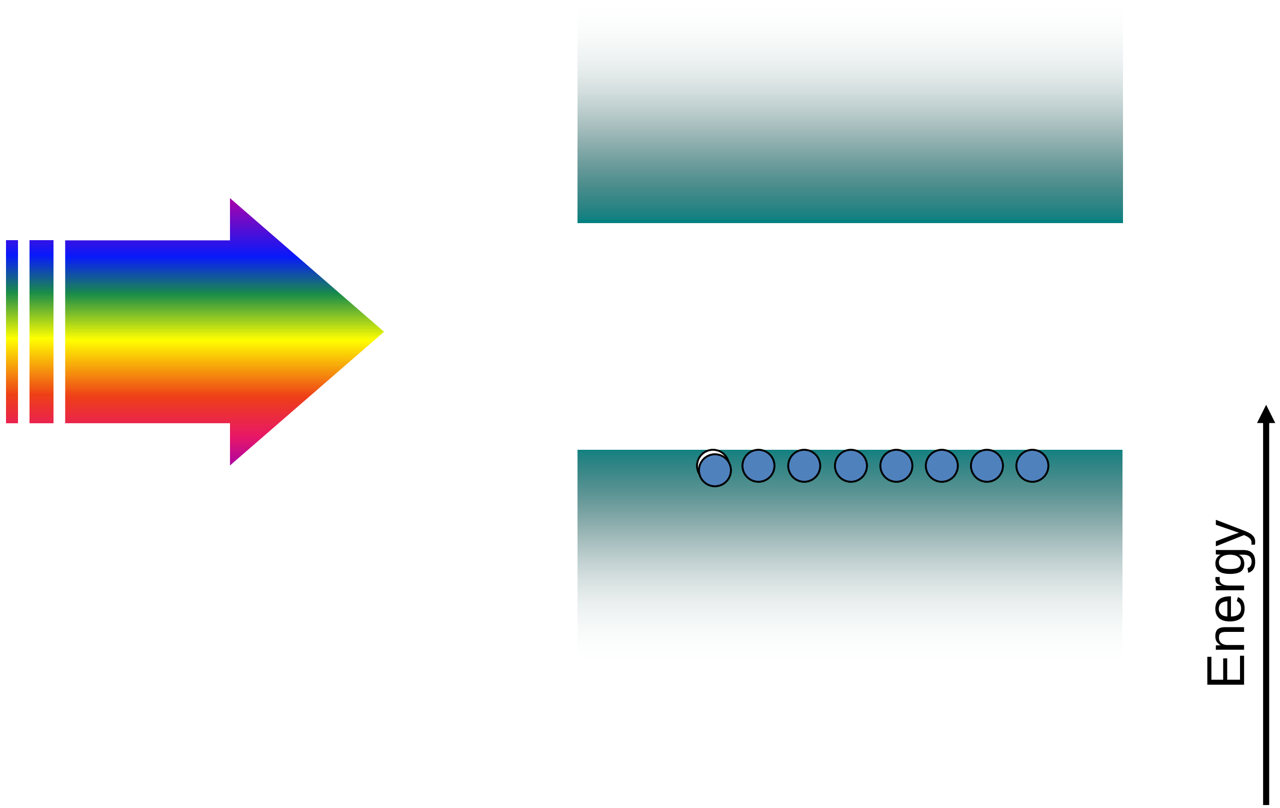






*A sidetrack: Photoelectric Effect

A “brother” of the PE effect: Photovoltaic Effect



Quantum Mechanics – basic concepts

2. Wave-particle dualism: Einstein, De Broglie

Light is a wave BUT can be emitted, absorbed, propagated in quanta (photons) with energy and momentum:

$$E = h\nu \qquad\qquad p = \frac{E}{c} = \frac{h}{\lambda}$$

Matter has a partcle-like properties, BUT also wave-like properties (matter waves*, de Broglie hypothesis):

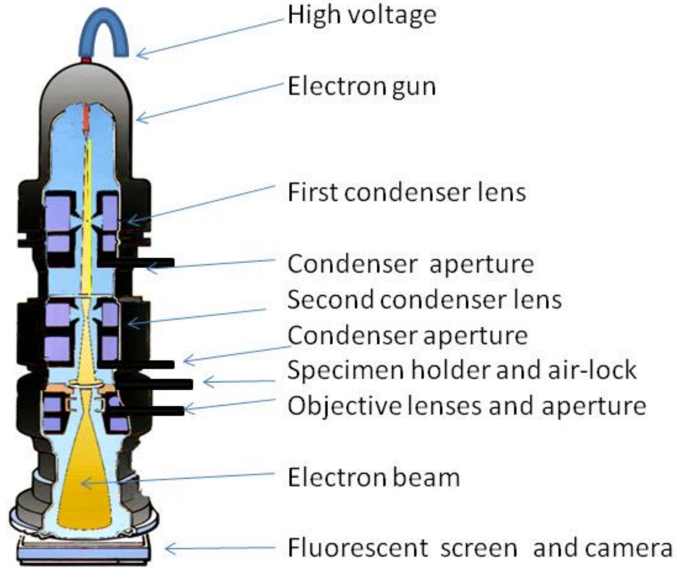
$$\lambda = \frac{h}{p}$$

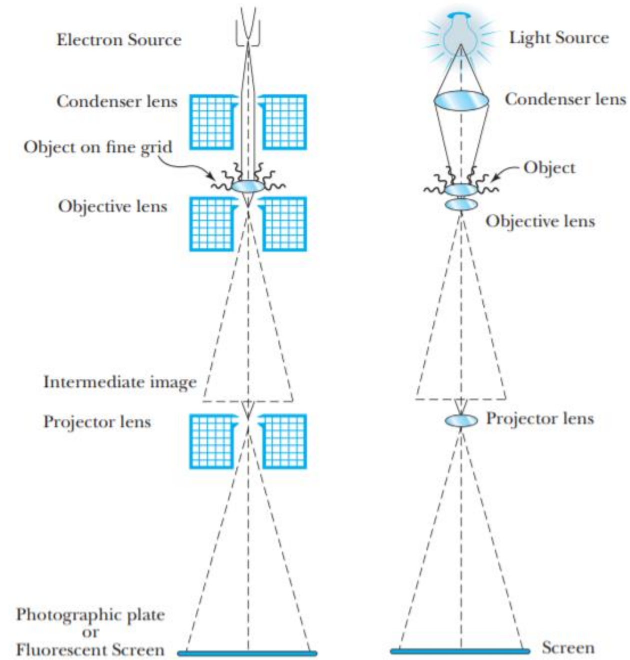
What is the wavelength of an electron?

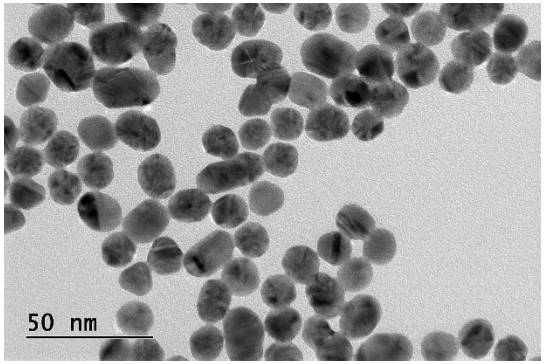
Excercises:

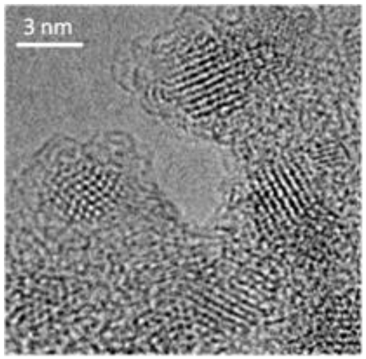
- Calculate the wavelength of an electron (algebraic formula)
- Calculate the wavelength of a “slow” electron (e.g. one accelerated by a $\Delta V = 54$ V)
- Read about Davisson and Germer’s experiment (they find that the electrons can diffract from metal surfaces → Experimental proof of matter waves)
- Calculate the wavelength of “fast” electrons (hint: account for the relativistic speed correction). Use the formula to estimate the error when neglecting relativistic effects for electrons accelerated by $\Delta V = 54$ MV

*Sidetrack:
Matter waves and electron microscopy



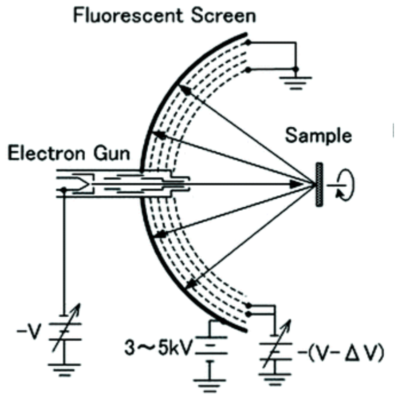


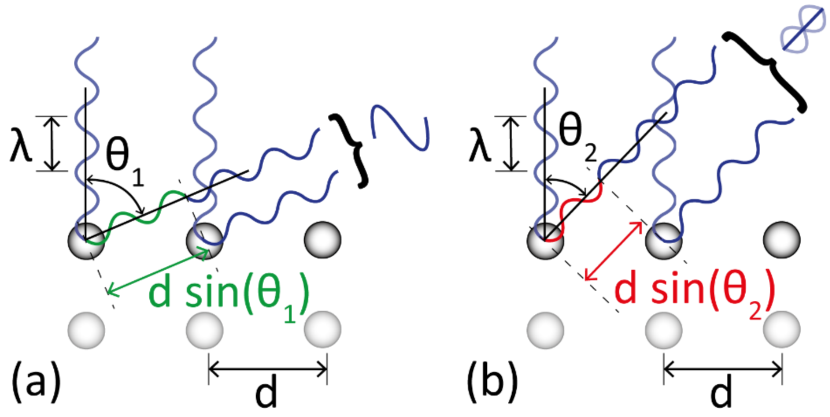


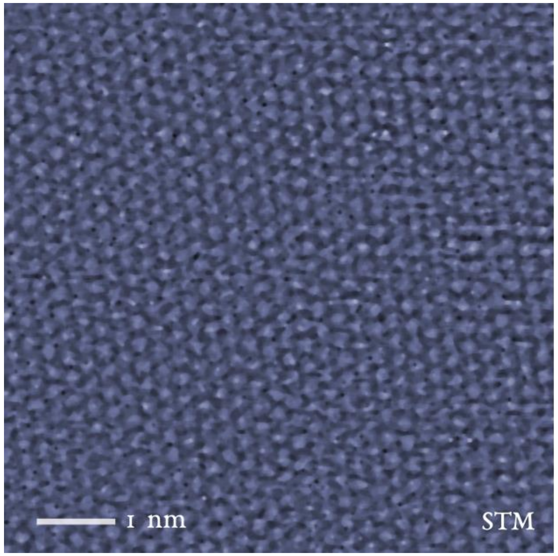


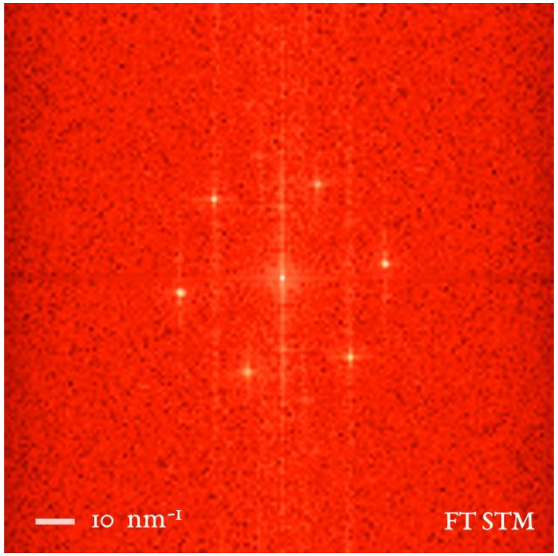
*Sidetrack: Matter waves and LEED

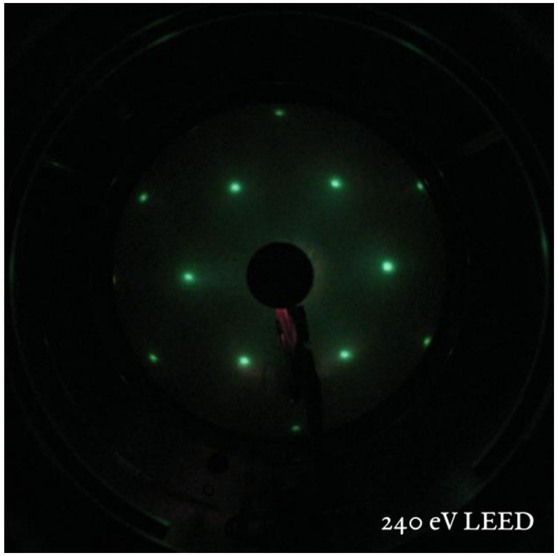
Thank you Davisson and Germer!







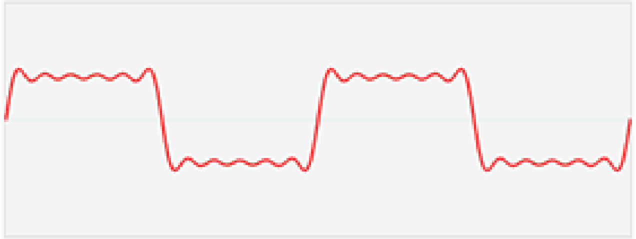




Sidetrack in a sidetrack: Fourier Analysis

Any function can be expressed as a **Fourier series**

$$s_N(x) = \frac{a_0}{2} + \sum_{n=1}^{N} \left(a_n \cos\left(\frac{2\pi n x}{P}\right) + b_n \sin\left(\frac{2\pi n x}{P}\right) \right)$$



Fourier coefficients

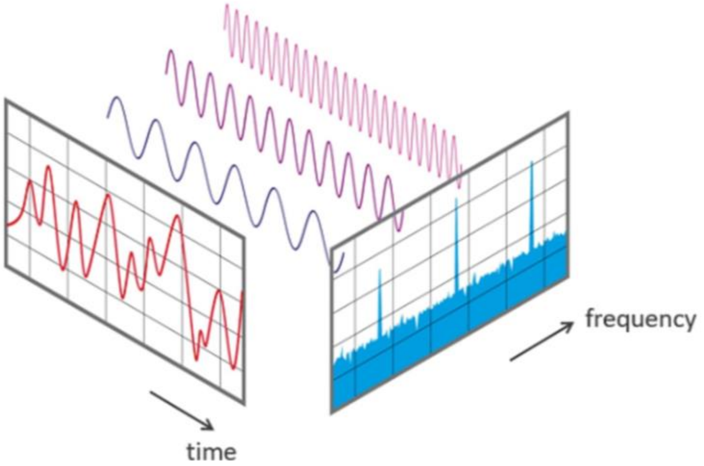
$$a_n = \frac{2}{P} \int_P s(x) \cdot \cos\left(2\pi x \tfrac{n}{P}\right) dx$$

$$b_n = \frac{2}{P} \int_P s(x) \cdot \sin\left(2\pi x \tfrac{n}{P}\right) dx.$$

Fourier transform can simplify the analysis
(e.g. FT-IR spectroscopy)

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

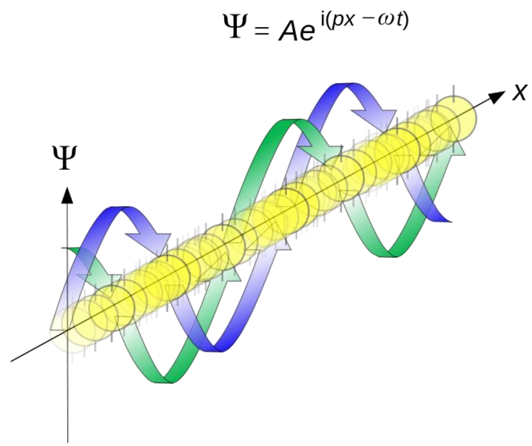
$$a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-ikx} dk$$



Quantum Mechanics – basic concepts

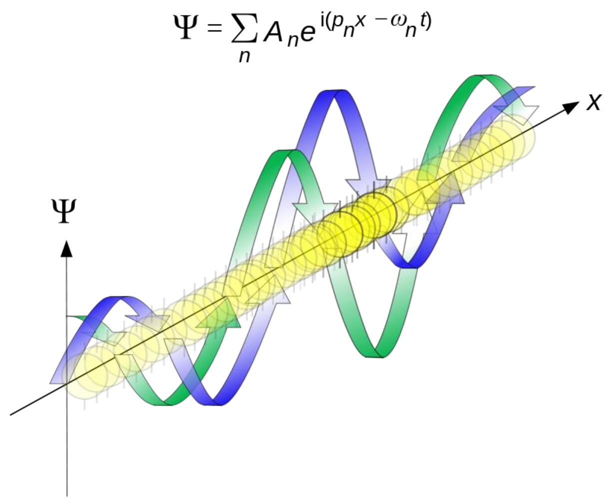
3. Matter waves and wave packets

Single plane wave



$v_p = \frac{\omega}{k}$

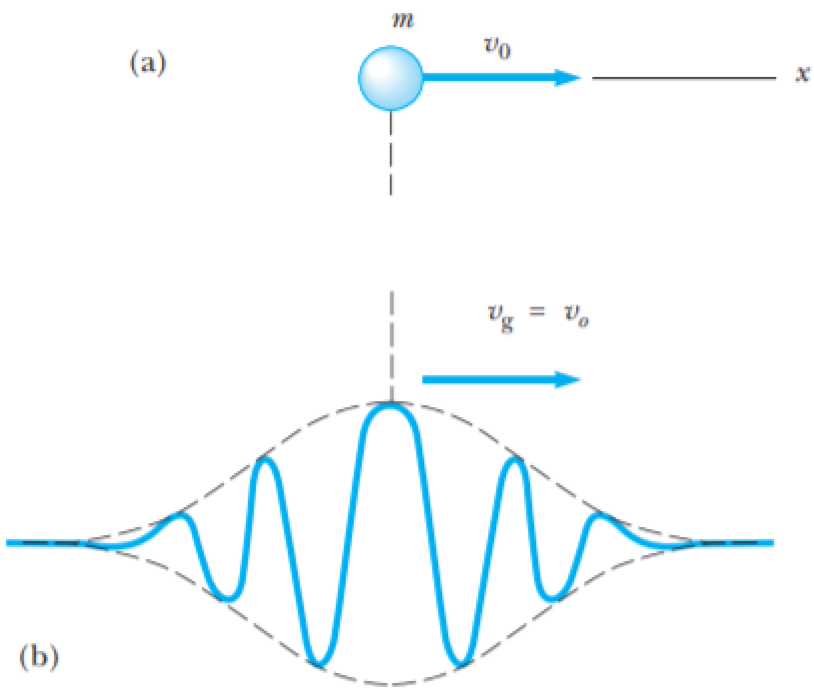
Wave packet



Example: two waves

Quantum Mechanics – basic concepts

3. Matter waves and wave packets



$$v_g = \frac{d\omega}{dk}\bigg|_{k_0} = v_p\Big|_{k_0} + k\frac{dv_p}{dk}\bigg|_{k_0}$$

Example: non relativistic particle
Homework: relativistic particle

The velocity of the particle is the group velocity of the wavepacket

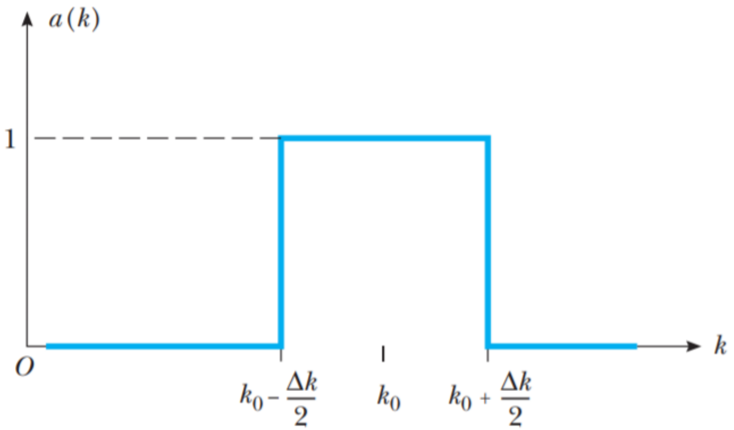
Quantum Mechanics – basic concepts

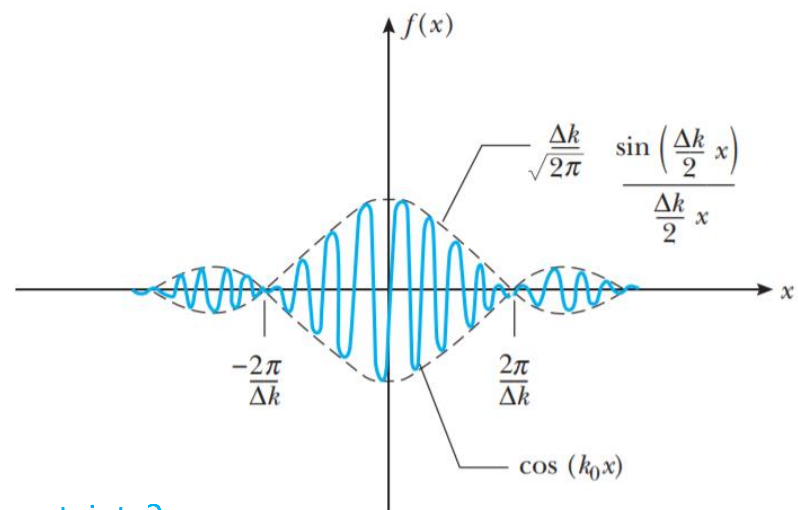
3. Matter waves and wave packets. Example: rectangular wavepacket

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

$$= \frac{1}{\sqrt{2\pi}} \int_{k_0-(\Delta k/2)}^{k_0+(\Delta k/2)} e^{ikx}\, dk =$$

$$= \frac{\Delta k}{\sqrt{2\pi}} \frac{\sin(\Delta k \cdot x/2)}{(\Delta k \cdot x/2)} e^{ik_0 x}$$

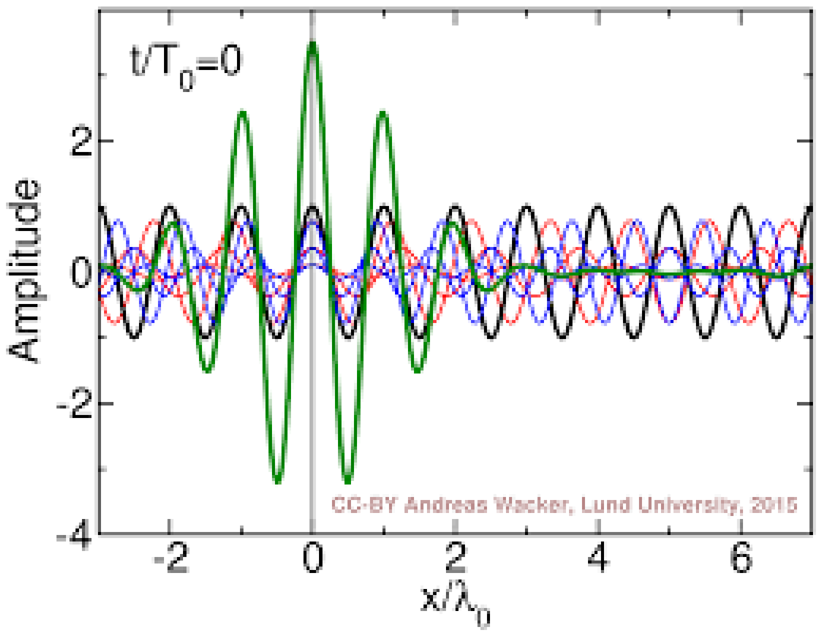




What is the uncertainty?

Quantum Mechanics – basic concepts

3. Matter waves and wave packets

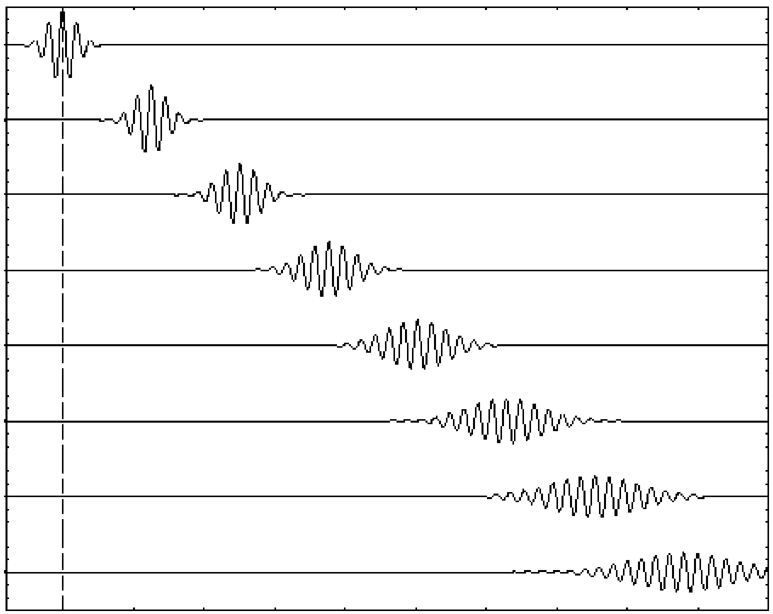


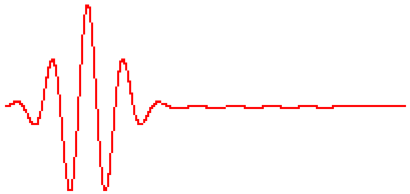
$$u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\; e^{i(kx-\omega(k)t)}\, dk$$

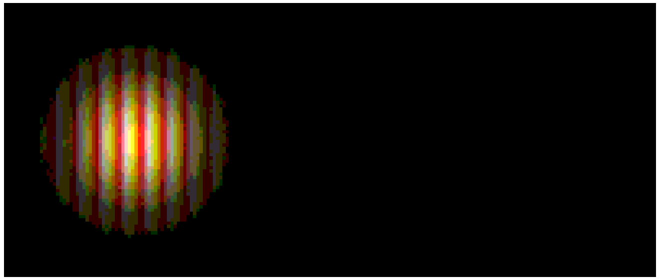
Quantum Mechanics – basic concepts

3. Matter waves and wave packets

Dispersive Wavepackets







Quantum Mechanics – basic concepts

3. Matter waves and wave packets

https://demonstrations.wolfram.com/WavepacketForAFreeParticle/

https://physics.nyu.edu/~ts2/Animation/quantum.html

https://www.ncnr.nist.gov/staff/dimeo/se_sim.html

Quantum mechanics – basic concepts

4. Uncertainty

$$\Delta p_x \, \Delta x \geq \frac{\hbar}{2} \qquad \Delta E \Delta t \geq \frac{\hbar}{2}$$