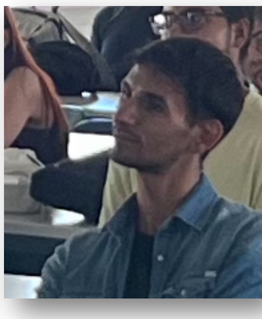
MSE 423 Fall 2025 – Week 1

WAVE MECHANICS

The mechanics of the quantum mechanics class: MSE 423 Team

- **Lectures: Tue 11am-1pm, Thu 2pm-3pm – in MXF-1 (for now)**
- **Exercises: Thu 3pm-4pm – in MXF-1 (for now)**
- **Office hours: Tue 1pm (ideally email first)**

Nicola Marzari nicola.marzari@epfl.ch
Binbin Liu binbin.liu@epfl.ch
Andrea Pintus andrea.pintus@epfl.ch
Luca Righetti luca.righetti@epfl.ch
Matteo Quinzi matteo.quinzi@epfl.ch



MSE 423 Practicals

- Moodle: https://moodle.epfl.ch/course/view.php?id=18242
- Google drive for the recordings (need to log in as EPFL): https://bit.ly/3JRNVN0
- Zoom: https://bit.ly/3Ka9hVQ

MOODLE	EPFL GOOGLE DRIVE	ZOOM
All class material	Archive of all zoom recordings (need to login with your EPFL account!)	Live broadcast

A brief history…

Education

- Laurea in Physics (University of Trieste, 1992)
- PhD in Physics (University of Cambridge, 1993-96)
- NSF Postdoc (Rutgers University, 1996-98)
- Research Scientist (Princeton University, 1999-01)

Professional

- Assistant Professor (MIT, 2001-05)
- Associate Professor (MIT, 2005-09)
- Toyota Chair of Materials Engineering (MIT, 2009-11)

- Statutory ("University") Chair of Materials Modelling (U. of Oxford, 2010-11)
- Director, Materials Modelling Laboratory (U. of Oxford, 2010-11)

- Chair, Theory and Simulation of Materials (EPFL, 2011-2026)
- Director, National Centre MARVEL for Materials Design and Discovery (2014-2026)
- Head, Laboratory of Materials Simulations, Paul Scherrer Institut (2021-2026)

- Cavendish Professor of Physics (University of Cambridge, 2025-onwards)

Textbook

A couple of useful texts:

- **Mortimer, *Physical Chemistry (Elsevier, 3rd Ed., 2008)***
- **Rolf E Hummel, *Electronic Properties of Materials,*** Springer (2011) (ISBN: 978-1-4419-8163-9 (Print) 978-1-4419-8164-6 (Online))

The last one is FREE to EPFL students as a PDF at http://link.springer.com: http://link.springer.com/book/10.1007/978-1-4419-8164-6

You can purchase a softcover from the same website for 25 CHF (but will not use it overly – relying mostly on readings that I will post).

Other (very good) textbooks

- **Bransden & Joachain, *Quantum Mechanics (Prentice Hall, 2nd Ed., 2000)***
- **Bransden & Joachain, *Physics of Atoms and Molecules (Prentice Hall, 2nd Ed., 2003)***
- **Ashcroft and Mermin, *Solid-state physics (Brooks/Cole, 1976)***
- **Kittel, *Introduction to solid-state physics (Wiley, 8th Ed., 2004)***

Oxford Masters Series (Oxford University Press)

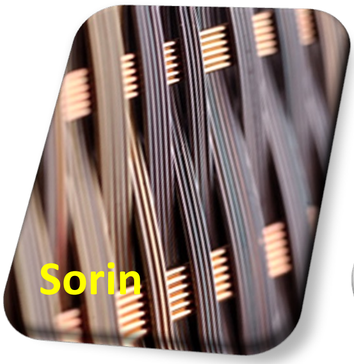
- **Singleton, *Band Theory and Electronic Properties of Solids***
- **Fox, *Optical Properties of Solids***
- **Dove, *Structure and Dynamics***
- **Blundell, *Magnetism in Condensed Matter***

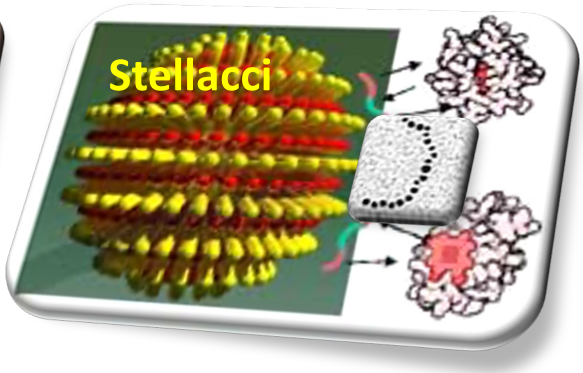
Homework (1 exercise per week, not graded) and written exam

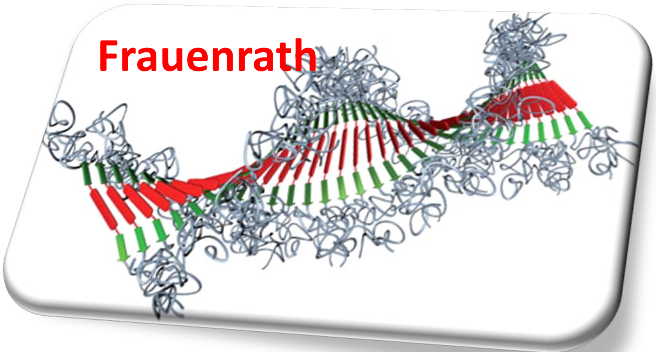
- Every Tue: exercise for the following week, and the solution for the current one, uploaded on Moodle
- Every Thu: solution for the current one discussed; you can work on the following one, and ask questions
- **We don't grade the homework.** You do it to understand you master the material.
- We will have a written exam in January – 3 hours, 4 question. Two theory questions, and two exercises. Closed book, you cannot have any material with you. We'll give you at the end of the class a list of the theory questions that could be asked. The exercises will closely follow the ones you did during the semester. If absent (justified) can take a oral exam later.

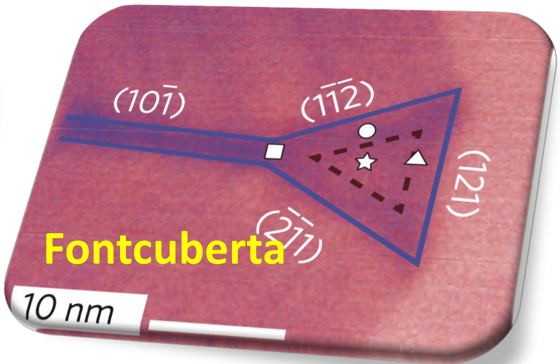
Physical Origin of Material Properties

Advanced materials' research



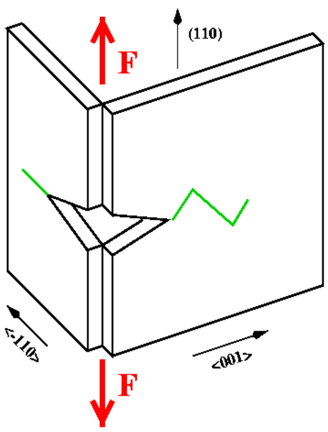


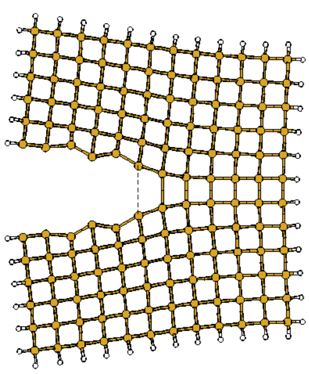


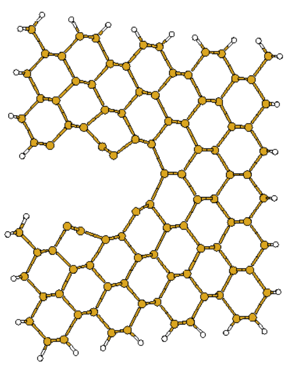


Why do we need quantum mechanics ?

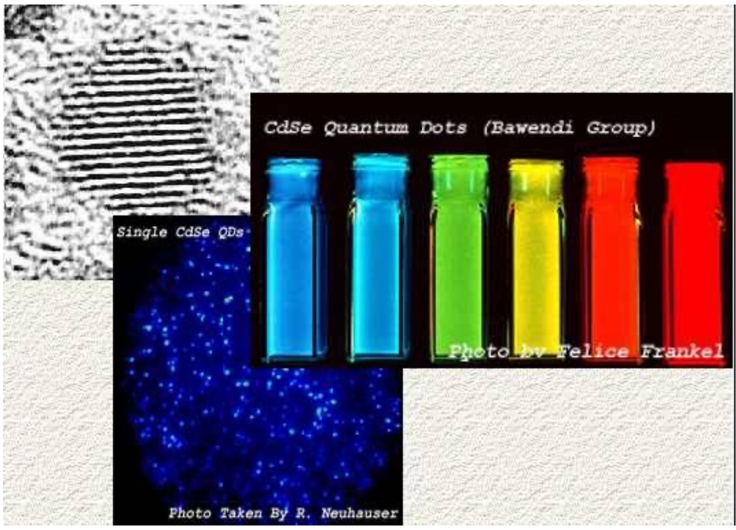
Structural properties (fracture in solids)







Electronic, optical, magnetic properties

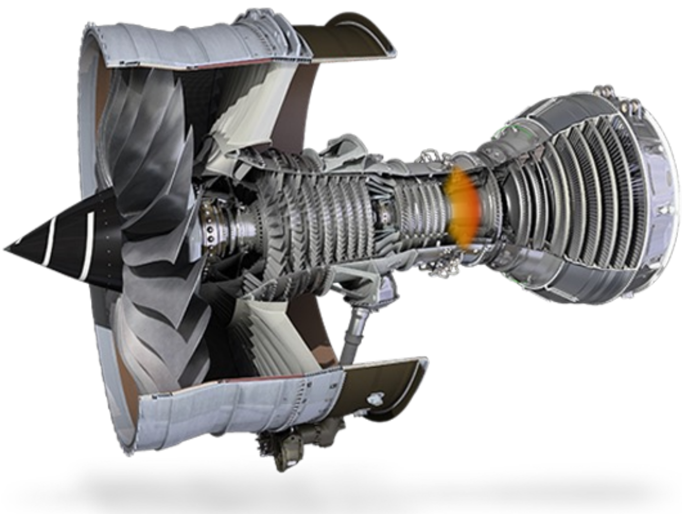


Changing the world…

…for better or for worse

A few easy pieces

Next time you fly

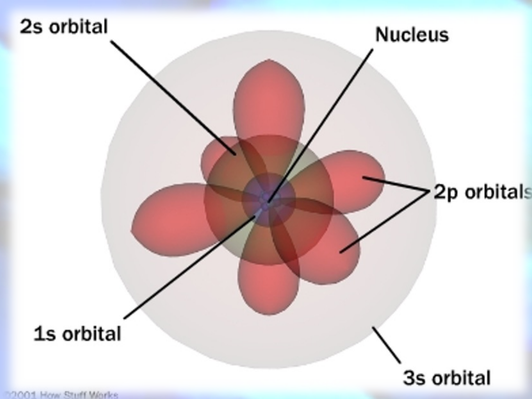


MSE 423 Fundamentals of Solid-state Materials - Nicola Marzari (EPFL, Fall 2025)

Meet Clara and Fritz

Standard Model of Matter

- Atoms are made by massive, point-like nuclei (protons+neutrons)
- Surrounded by tightly bound, rigid shells of core electrons
- Bound together by a glue of valence electrons (gas vs. atomic orbitals)



Some energy scales

- An electron in a 1V potential = 1 eV = 1.602×10^{-19} J
- Energy at our living conditions (300 K): 0.04 eV
  (kinetic energy of an atom in an ideal gas).
- Hydrogen bond: 0.29 eV. Cohesive energy of silicon 4.6 eV/atom.
  Diamond 7.4 eV/atom.
- Energy of visible light: 1.6-3.1 eV.
- Binding energy of an electron to a proton (hydrogen):
  13.6058 eV = 1 Ry (rydberg) = 0.5 Ha (hartree) = 0.5 atomic units

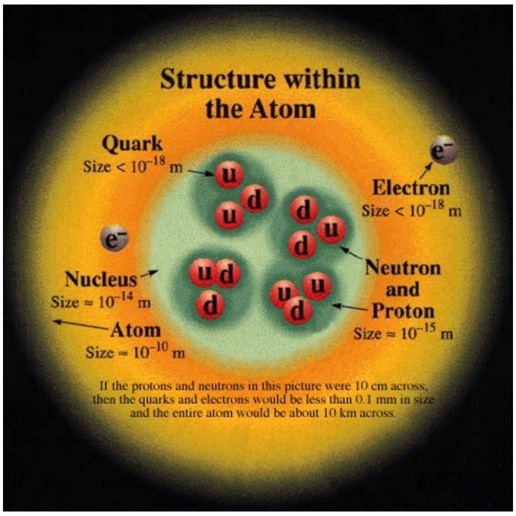
From Classical to Quantum

Round Up the Usual Suspects

- Particles and electromagnetic fields
- Forces
- Dynamics

Particles

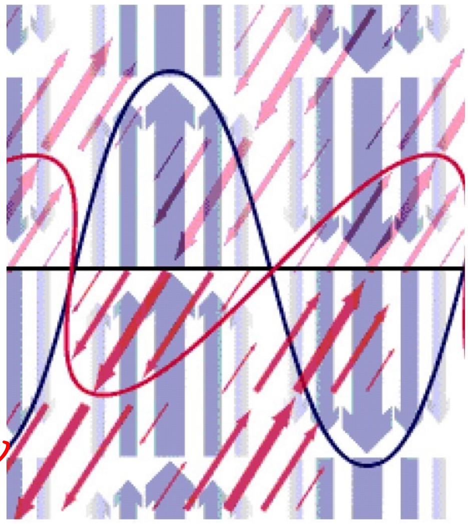
- Electrons
- Nuclei (protons, neutrons)
- What are their equations of motion?



Fields

- Electric and magnetic fields
- What are their equations of motion?

J.C. MAXWELL ~1860-1870



Electromagnetic Waves / Photons

$$E = h\nu = h\frac{c}{\lambda} = kT$$

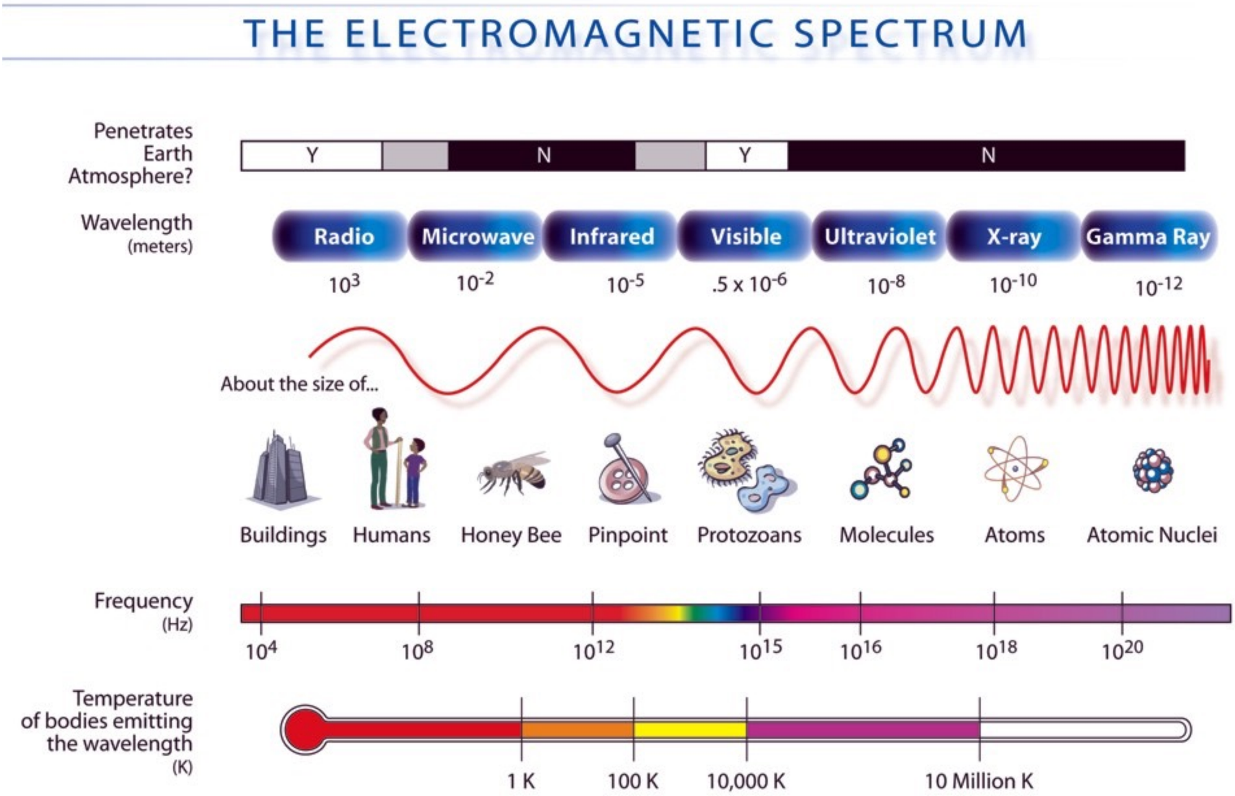
h is Planck's constant = 6.626 10^{-34} J s

c is the speed of light = 299 792 458 m / s

k is Boltzmann's constant = 1.381 10^{-23} J/K

(also, 1eV = $1.602176565\times10^{-19}$ J)

E is the energy (J), ν is the frequency (1/s), λ the wavelength (m)



Examples: http://imagers.gsfc.nasa.gov/ems/ems.html

Forces

- Electromagnetic interactions
- (Gravity, electroweak, strong)

Dynamics of a Particle

$$m\frac{d^2\vec{r}}{dt^2} = F(\vec{r}) \longrightarrow \begin{matrix}\vec{r}(t)\\ \vec{v}(t)\end{matrix}$$

The sum of the kinetic and potential energy (E=T+V) is conserved

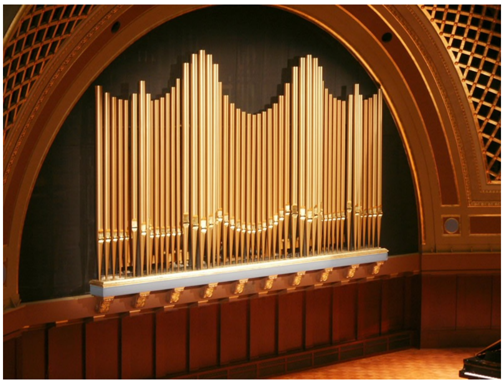
Dynamics of a Particle

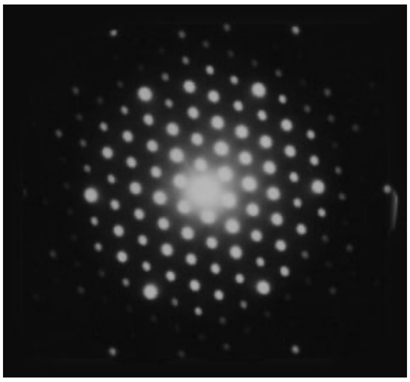
$$m\frac{d^2\vec{r}}{dt^2} = F(\vec{r}) \longrightarrow \begin{matrix}\vec{r}(t)\\ \vec{v}(t)\end{matrix}$$

The sum of the kinetic and potential energy (E=T+V) is conserved

Wave-particle Duality

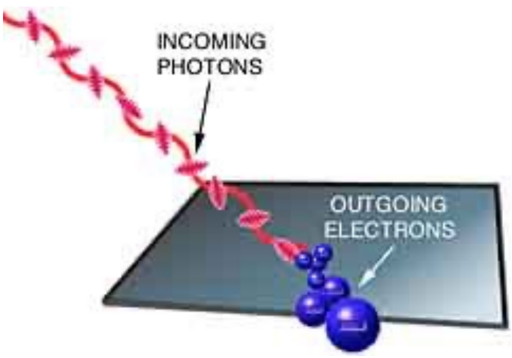
- Particles have wave-like properties:
  - Quantum mechanics: Electrons in atoms are standing waves – just like the harmonics of an organ pipe
  - Electrons beams can be diffracted, and we can see the fringes (Davisson and Germer, at Bell Labs in 1926…)

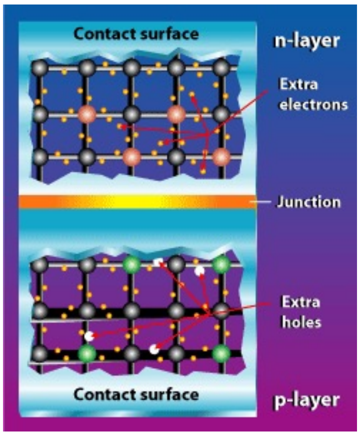




Wave-particle Duality

- *Waves have particle-like properties:*
  - *Photoelectric effect: quanta (photons) are exchanged discretely*
  - *Energy spectrum of an incandescent body looks like a gas of very hot particles*

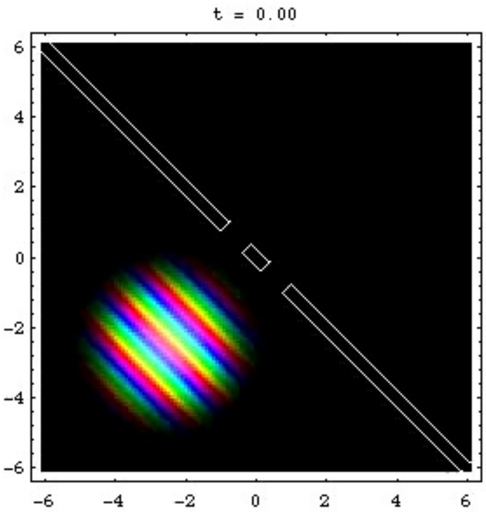




When is a particle like a wave ?

Wavelength • momentum = Planck

L. DE BROGLIE



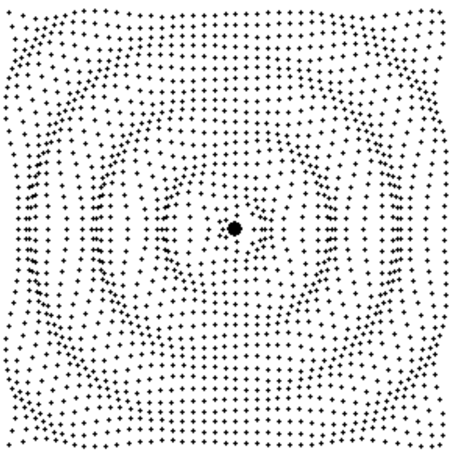
↕

$$\lambda \bullet p = h$$

(h = 6.626 x 10^{-34} J s = 2π a.u.)

http4://www.kfunigraz.ac.at/imawww/vqm/

Description of a Wave



The wave is an excitation (a vibration): We need to know the amplitude of the excitation at every point and at every instant

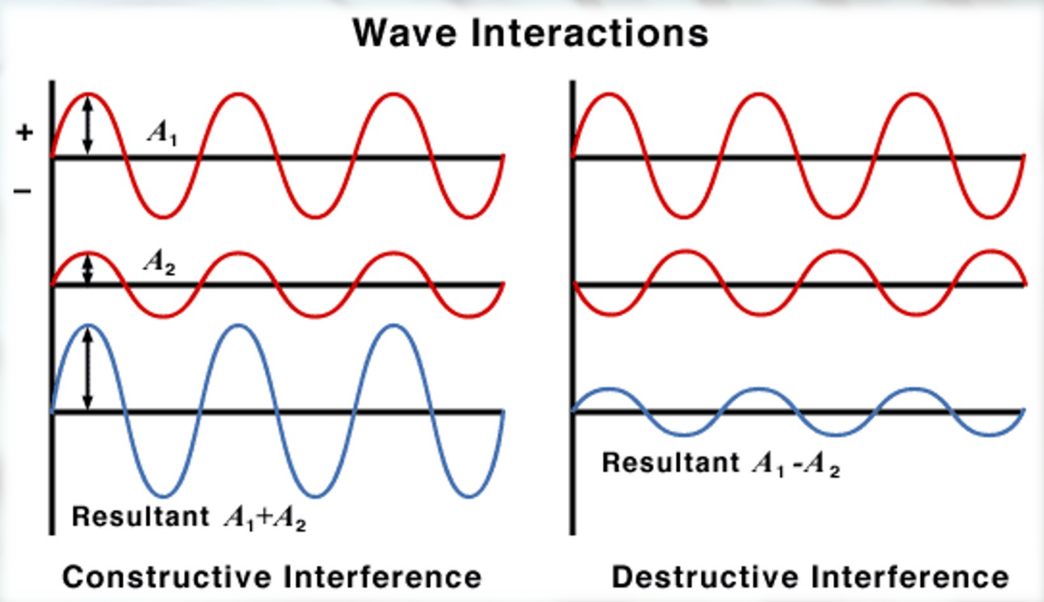
$$\Psi = \Psi(\vec{r}, t)$$

Description of a Wave

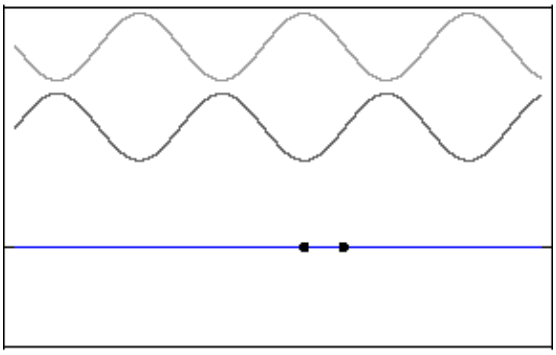
The wave is an excitation (a vibration): We need to know the amplitude of the excitation at every point and at every instant

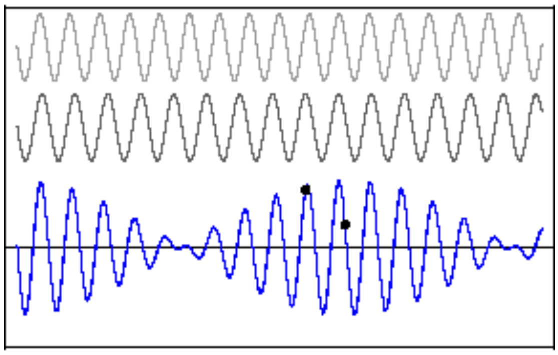
$$\Psi = \Psi(\vec{r}, t)$$

Principle of linear superposition

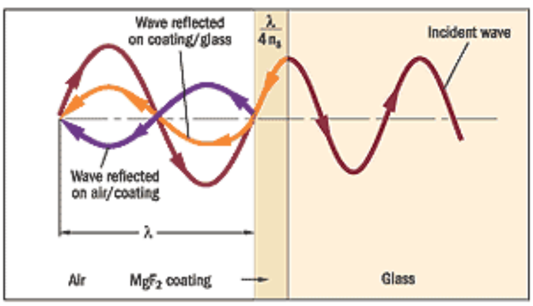


Interference in Action



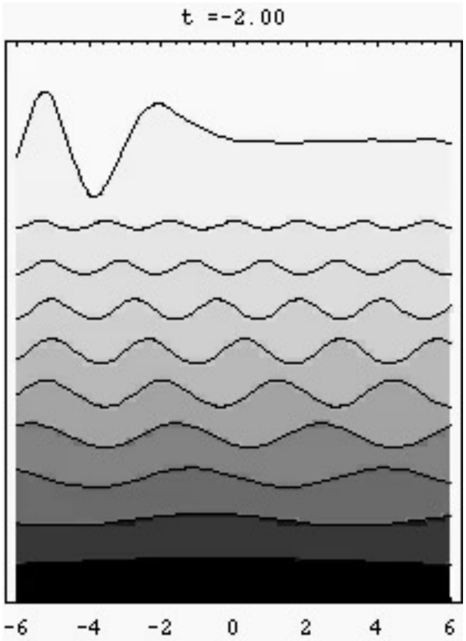


Interference in Action



Source: Carl Zeiss Inc.

Also: decomposition of arbitrary functions into sines/cosines



AROSA (GRAUBÜNDEN/GRISONS), 27th DECEMBER 1925

At the moment I am struggling with a new atomic theory. I am very optimistic about this thing and expect that if I can only... solve it, it will be very beautiful.

Erwin Schrödinger

Time-dependent Schrödinger's equation

(Newton's 2nd law for quantum objects)

$\hbar = \frac{h}{2\pi}$ (=1 a.u.)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + \mathrm{V}(\vec{r},t)\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

MASS OF e^-

$\Psi(\vec{r},t)$ $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

1925-onwards: E. Schrödinger (wave equation), W. Heisenberg (matrix formulation), P.A.M. Dirac (relativistic)

Plane waves as free particles

$\Psi(\vec{r},t) = A\exp[i(\vec{k}\cdot\vec{r} - \omega t)]$ satisfies the wave equation for a free particle

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

(provided $E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$)

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right] e^{i\vec{k}\cdot\vec{r}} A e^{-i\omega t} = i\hbar A e^{i\vec{k}\cdot\vec{r}} \frac{\partial}{\partial t} e^{-i\omega t}$$

$e^{i(k_x x + k_y y + k_z z)}$

$$-\frac{\hbar^2}{2m}\left[(ik_x)^2 e^{i\vec{k}\cdot\vec{r}} + (ik_y)^2 e^{i\vec{k}\cdot\vec{r}} + (ik_z)^2 e^{i\vec{k}\cdot\vec{r}}\right] e^{-i\omega t} = i\hbar e^{i\vec{k}\cdot\vec{r}} (-i\omega) e^{-i\omega t}$$

$$+\frac{\hbar^2}{2m}\left[+k_x^2 + k_y^2 + k_z^2\right] = i\hbar(+i\omega) = +\hbar\omega$$

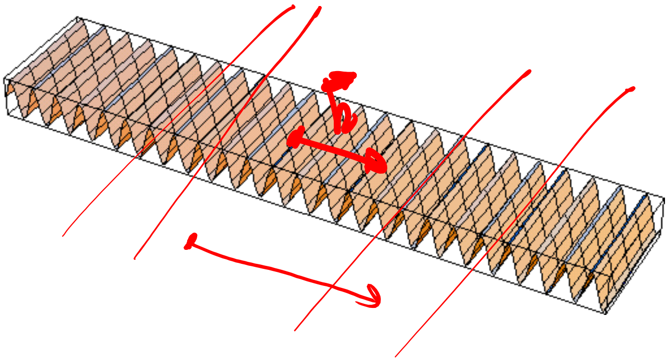
Plane waves as free particles

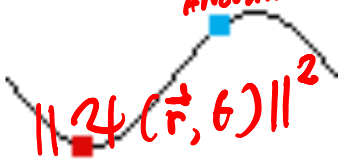
$$\int_V dr\, \psi^*(\vec{r},t)\,\psi(\vec{r},t) = 1$$

$$\Psi(\vec{r},t) = A\exp[i(\vec{k}\cdot\vec{r}-\omega t)]$$

WAVEVECTOR

ANGULAR FREQUENCY





$$\|\psi(\vec{r},t)\|^2$$