

MSE 423 Fall 2025 – Week 1

# WAVE MECHANICS



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

## 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**  
**Binbin Liu**  
**Andrea Pintus**  
**Luca Righetti**  
**Matteo Quinzi**

[nicola.marzari@epfl.ch](mailto:nicola.marzari@epfl.ch)  
[binbin.liu@epfl.ch](mailto:binbin.liu@epfl.ch)  
[andrea.pintus@epfl.ch](mailto:andrea.pintus@epfl.ch)  
[luca.righetti@epfl.ch](mailto:luca.righetti@epfl.ch)  
[matteo.quinzi@epfl.ch](mailto:matteo.quinzi@epfl.ch)



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# 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

All class material



## EPFL GOOGLE DRIVE

Archive of all zoom recordings  
(need to login with your EPFL account!)



## ZOOM

Live broadcast



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## 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)

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# Rolf E. Hummel **Textbook**

A couple of useful texts:

- Mortimer, *Physical Chemistry (Elsevier, 3<sup>rd</sup> 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, 2<sup>nd</sup> Ed., 2000)*
- Bransden & Joachain, *Physics of Atoms and Molecules (Prentice Hall, 2<sup>nd</sup> Ed., 2003)*
- Ashcroft and Mermin, *Solid-state physics (Brooks/Cole, 1976)*
- Kittel, *Introduction to solid-state physics (Wiley, 8<sup>th</sup> 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*

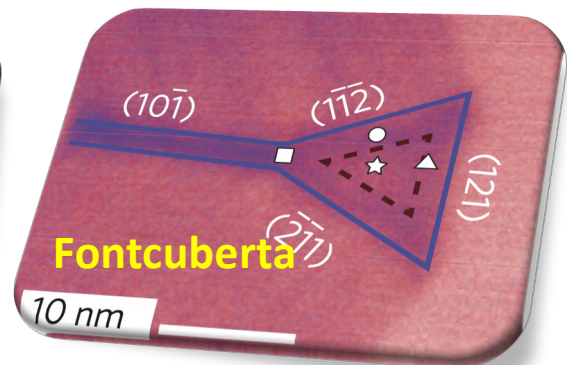
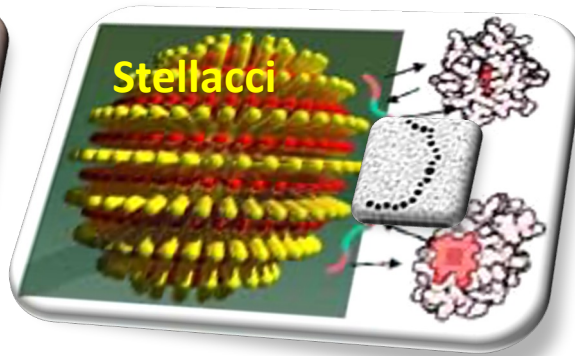
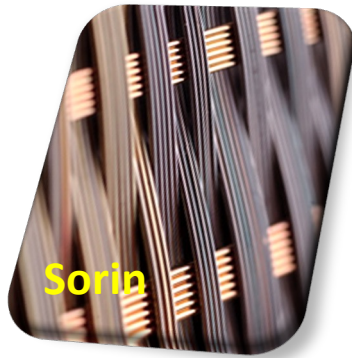
# Homework (1 exercise per week, not graded) and written exam

- 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.**

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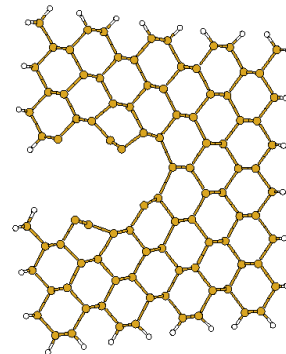
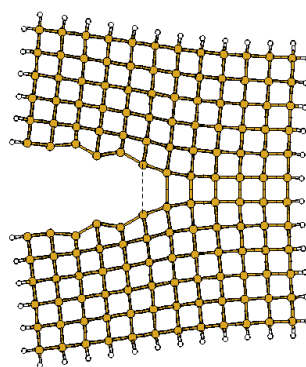
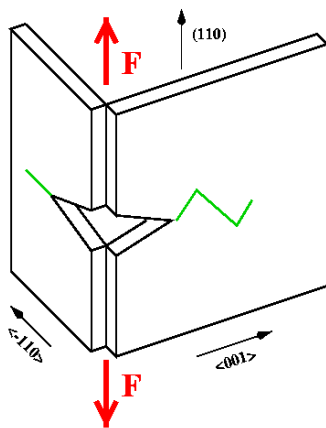
# Advanced materials' research



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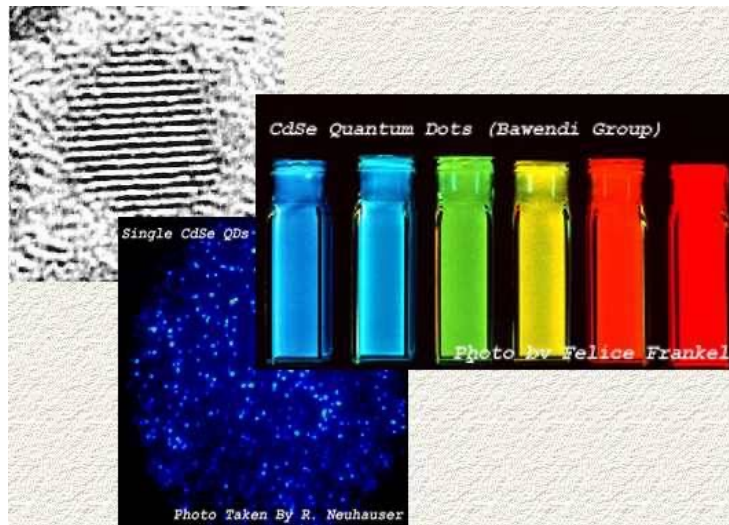
## Why do we need quantum mechanics ?

Structural properties (fracture in solids)



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# Electronic, optical, magnetic properties



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Changing the world...

...for better or for worse

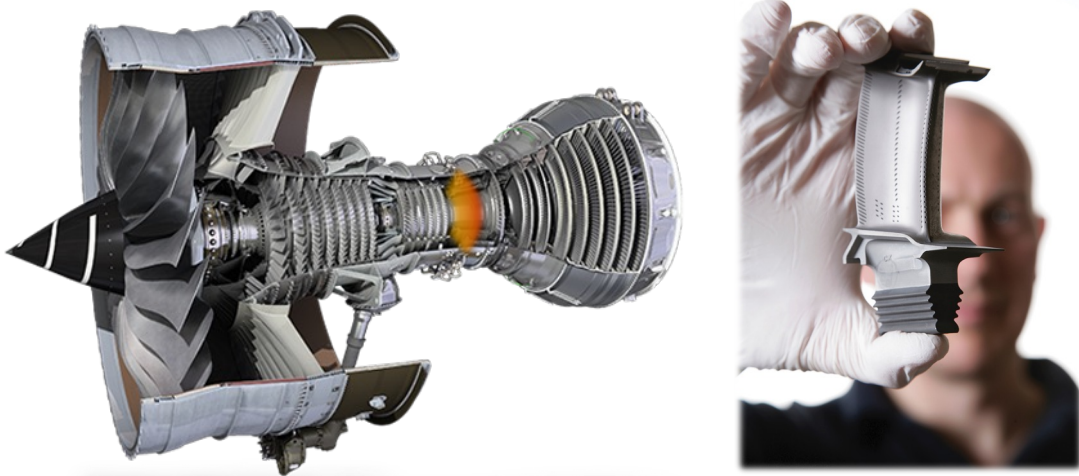
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# A few easy pieces



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# Next time you fly



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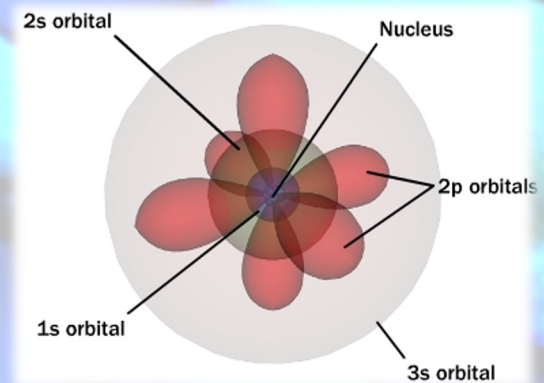
# Meet Clara and Fritz



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## 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)



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# Some energy scales

- An electron in a 1V potential = 1 eV =  $1.602 \times 10^{-19}$  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**

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## From Classical to Quantum

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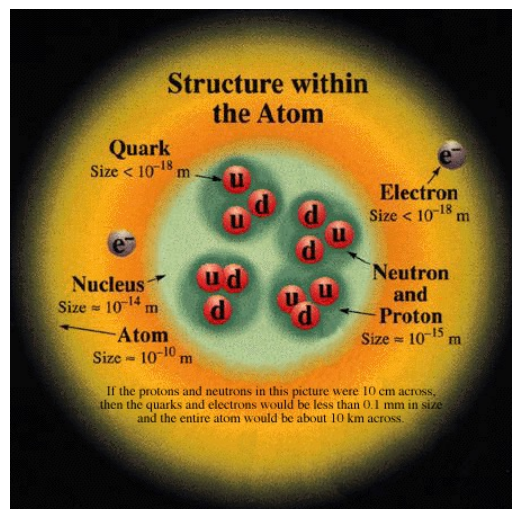
# Round Up the Usual Suspects

- Particles and electromagnetic fields
- Forces
- Dynamics

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## Particles

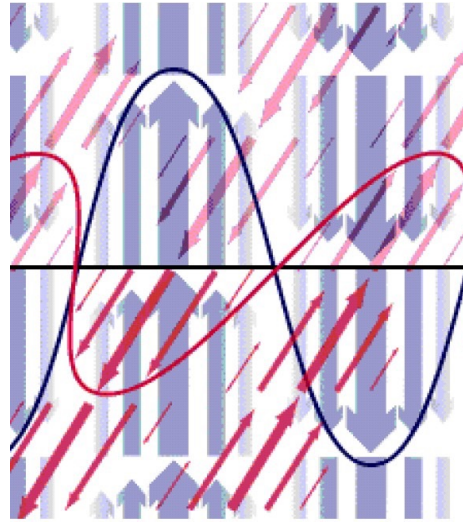
- Electrons
- Nuclei (protons, neutrons)
- What are their equations of motion?



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# Fields

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



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## Electromagnetic Waves / Photons

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

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

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

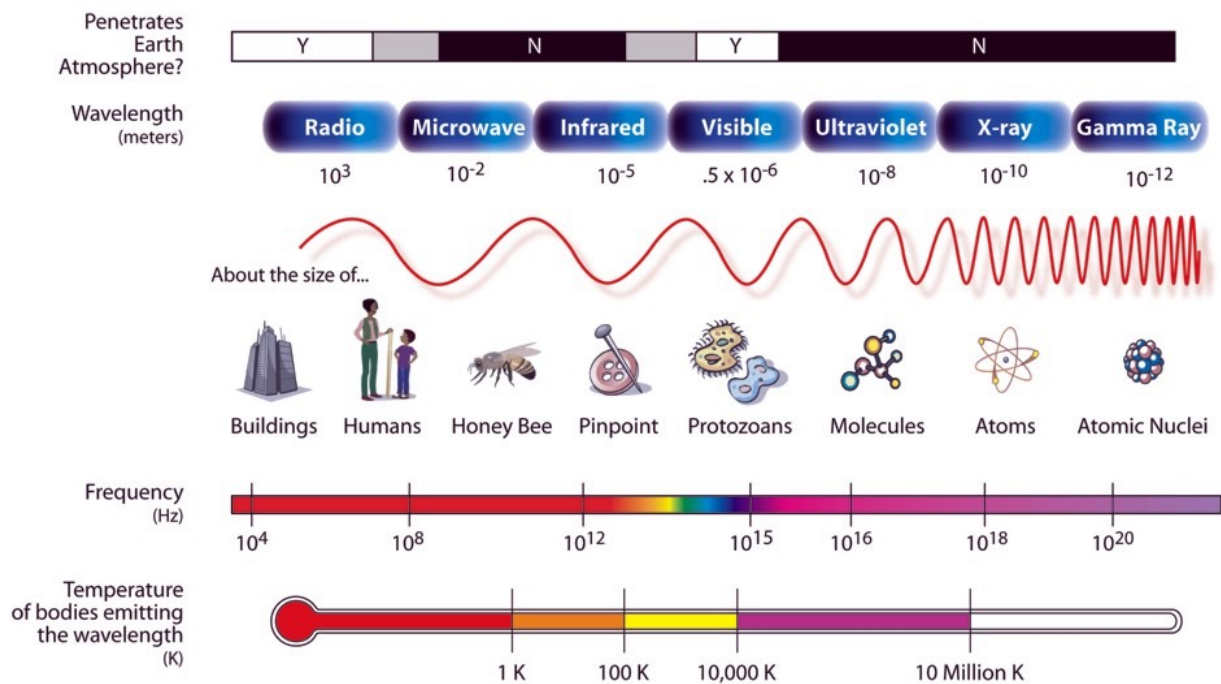
$k$  is Boltzmann's constant =  $1.381 \cdot 10^{-23}$  J/K

(also, 1eV =  $1.602176565 \cdot 10^{-19}$  J)

$E$  is the energy (J),  $\nu$  is the frequency (1/s),  $\lambda$  the wavelength (m)

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# THE ELECTROMAGNETIC SPECTRUM



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

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## Forces

- Electromagnetic interactions
- (Gravity, electroweak, strong)

## Dynamics of a Particle

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

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



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## Dynamics of a Particle

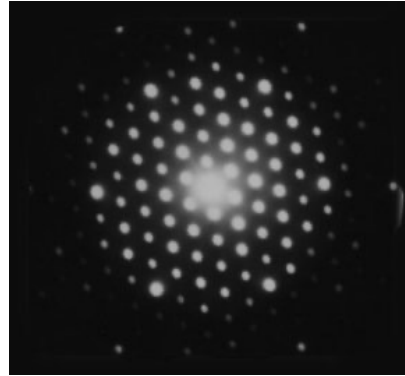
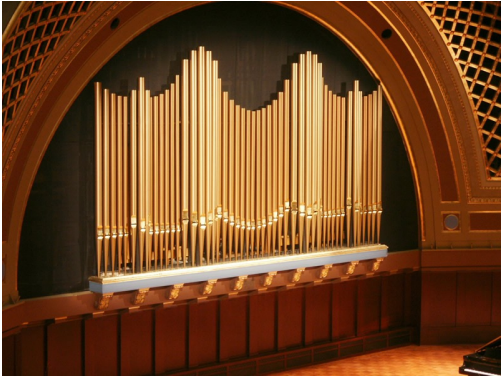
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# Wave-particle Duality

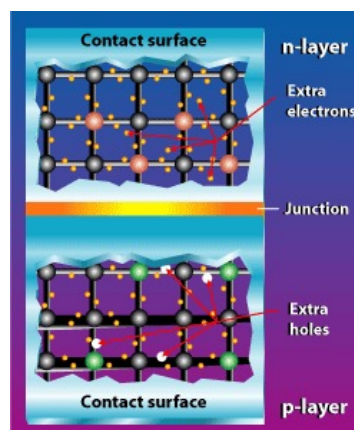
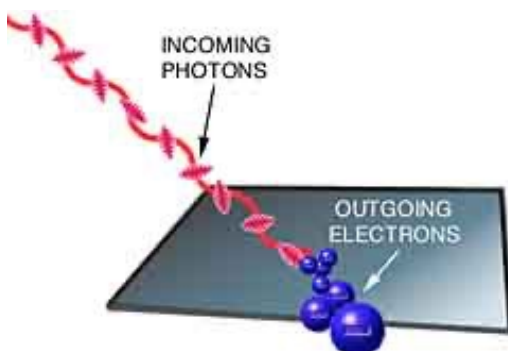
- Particles have wave-like properties:
  - Quantum mechanics: Electrons in atoms are standing waves – just like the harmonics of an organ pipe
  - Electrons beams can be diffracted, and we can see the fringes (Davisson and Germer, at Bell Labs in 1926...)



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# Wave-particle Duality

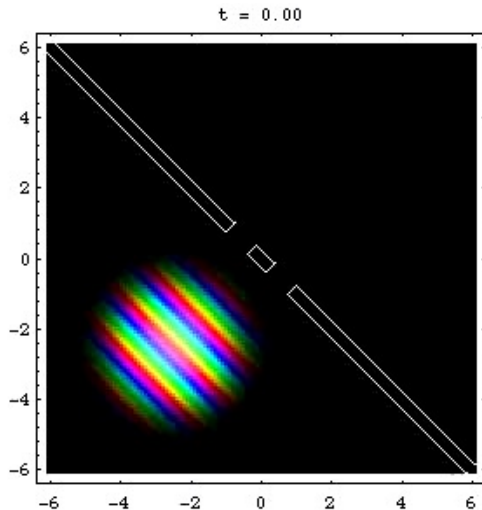
- *Waves have particle-like properties:*
  - *Photoelectric effect: quanta (photons) are exchanged discretely*
  - *Energy spectrum of an incandescent body looks like a gas of very hot particles*



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# When is a particle like a wave ?

Wavelength • momentum = Planck



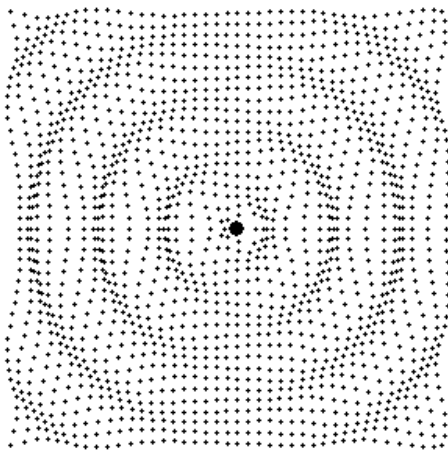
$$\lambda \cdot p = h$$

(  $h = 6.626 \times 10^{-34} \text{ J s} = 2\pi \text{ a.u.}$  )

<http://www.kfunigraz.ac.at/imawww/vqm/>

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## 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

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

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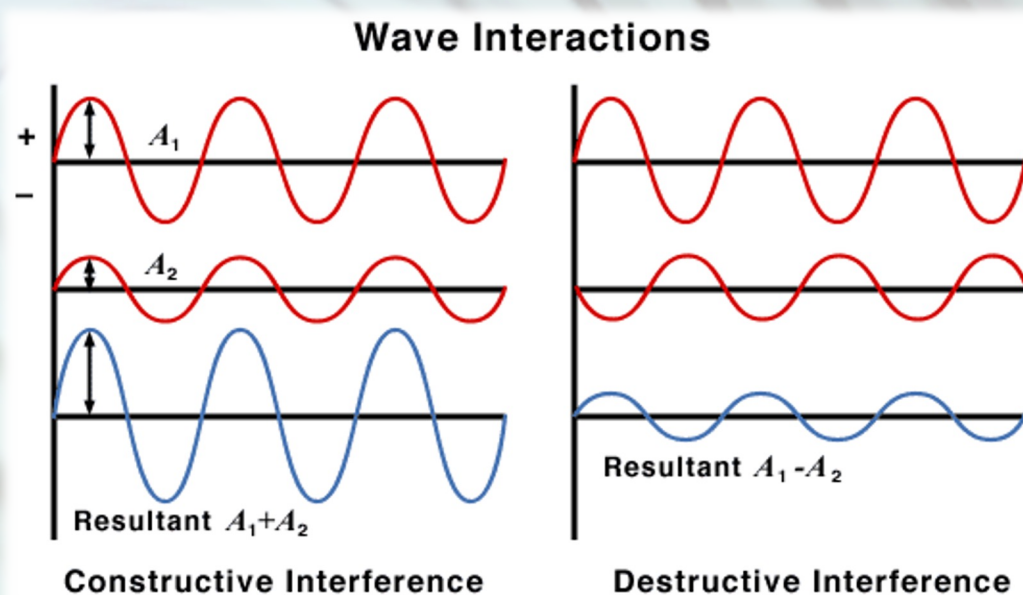
# Description of a Wave

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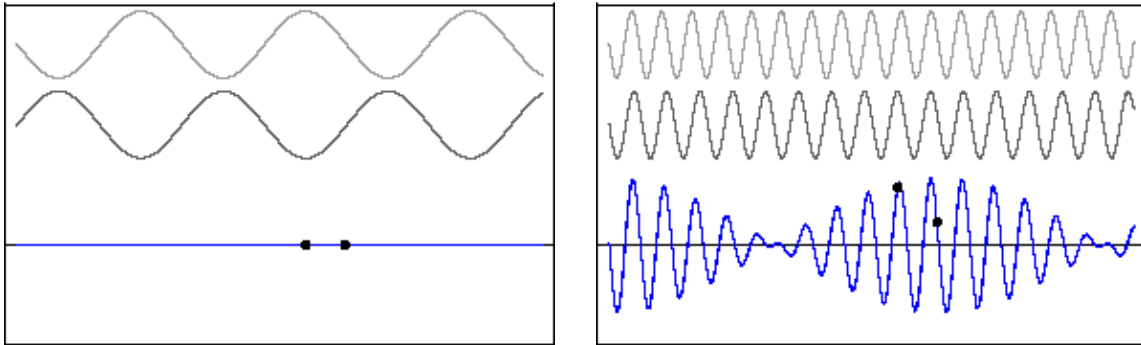
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## Principle of linear superposition



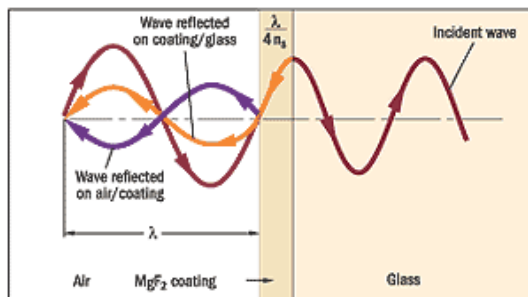
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# Interference in Action



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# Interference in Action

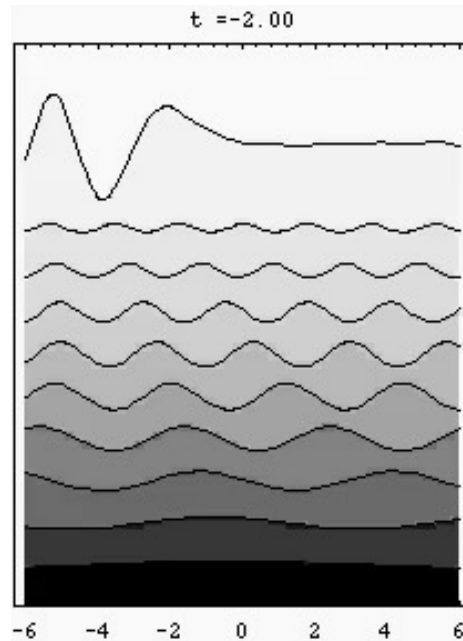


Source: Carl Zeiss Inc.



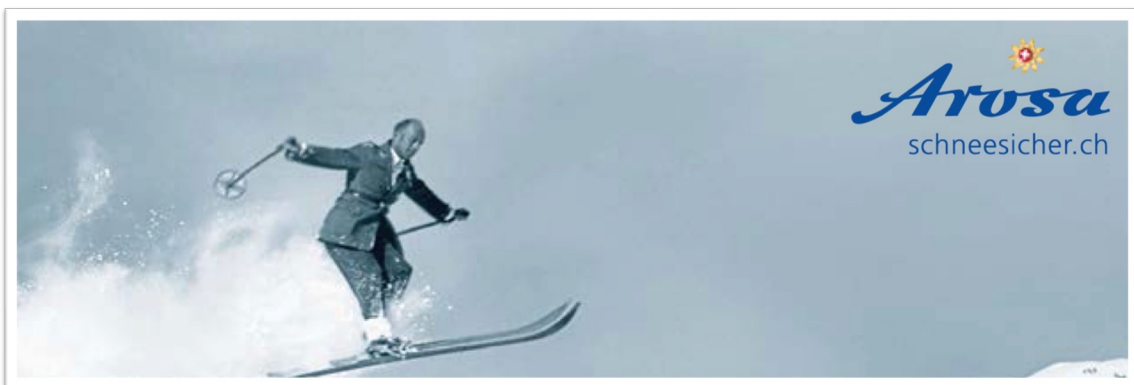
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## Also: decomposition of arbitrary functions into sines/cosines



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## AROSA (GRAUBÜNDEN/GRISONS), 27<sup>th</sup> 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*

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# Time-dependent Schrödinger's equation

(Newton's 2<sup>nd</sup> law for quantum objects)

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



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

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## Plane waves as free particles

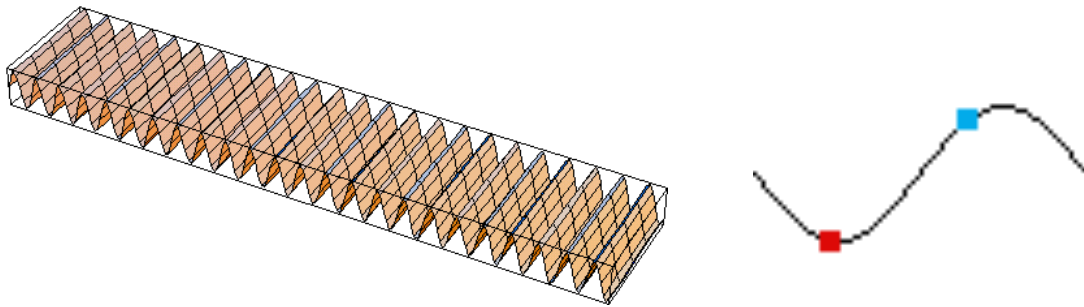
$\Psi(\vec{r},t) = A \exp[i(\vec{k} \cdot \vec{r} - \omega t)]$  satisfies the wave equation for a free particle

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} \quad (\text{provided } E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} )$$

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## Plane waves as free particles

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



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## Stationary Schrödinger's Equation (I)

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

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# Stationary Schrödinger's Equation (II)

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \varphi(\vec{r}) = E\varphi(\vec{r})$$