

WAVE MECHANICS



MSE 423 Fundamentals of Solid-state Materials - Nicola Marzari (EPFL, Fall 2024)

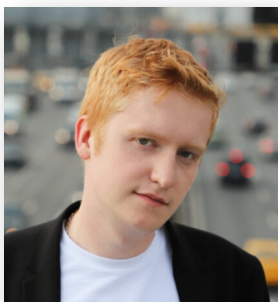
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The mechanics of the quantum mechanics class: MSE 423 Team

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

Nicola Marzari
Alexander Poliukhin
Luca Righetti
Matteo Quinzi

nicola.marzari@epfl.ch
aleksandr.poliukhin@epfl.ch
luca.righetti@epfl.ch
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/4eiOlpp>
- Zoom: <https://bit.ly/3XzZHQp>

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-onwards)
- Director, National Centre MARVEL for Materials Design and Discovery (2014-onwards)
- Head, Laboratory of Materials Simulations, Paul Scherrer Institut (2021-onwards)

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Rolf E. Hummel 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).

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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*

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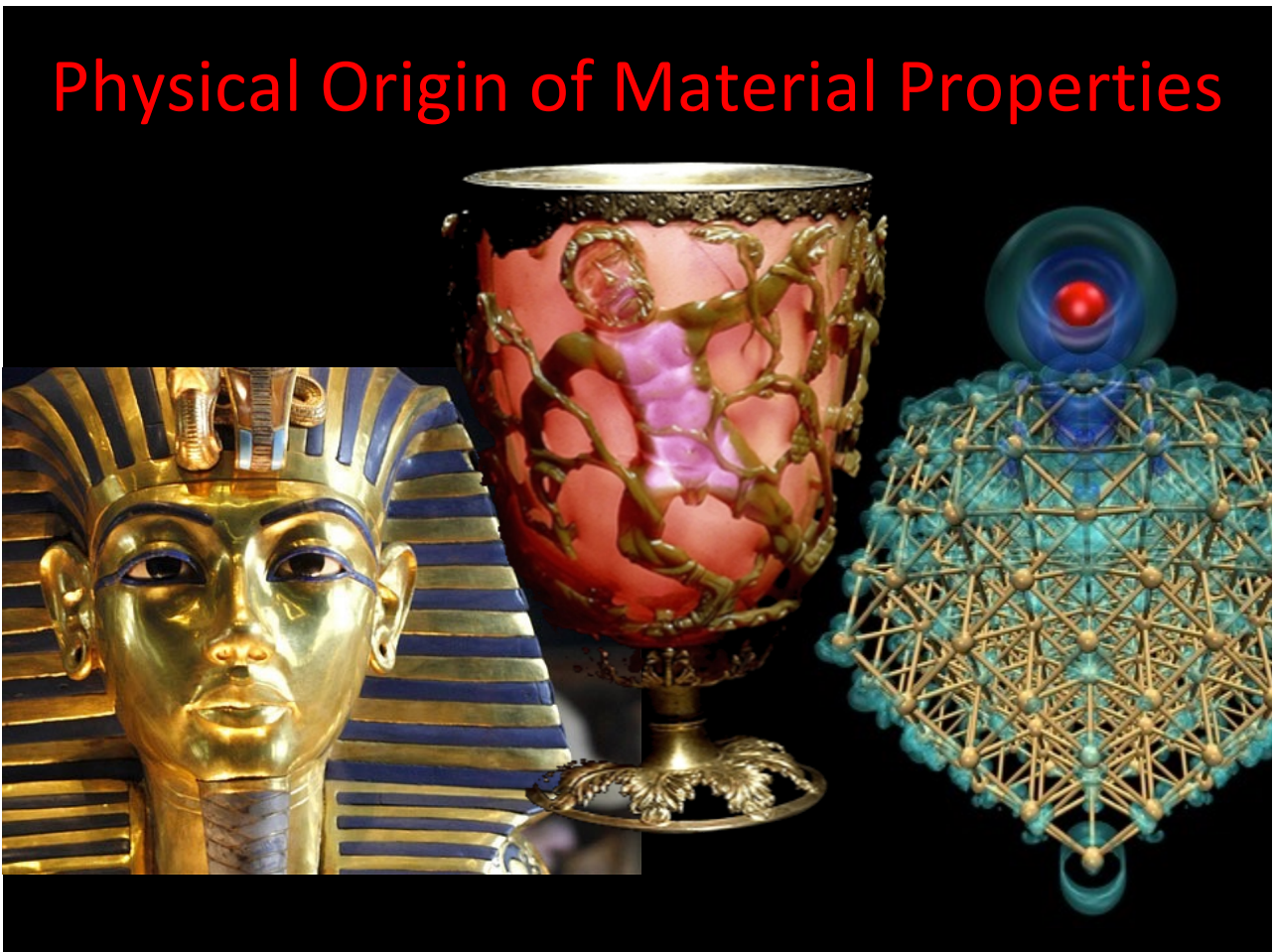
Homework (1 exercise per week, not graded) and written exam

- 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.

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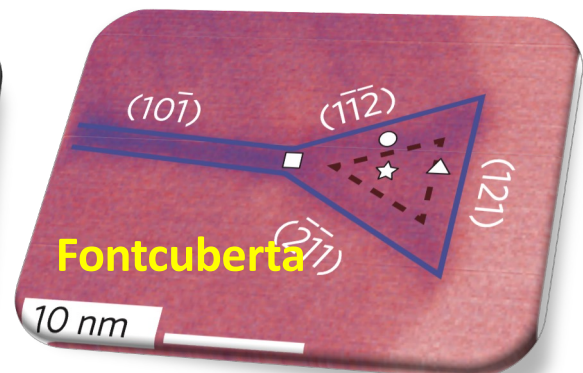
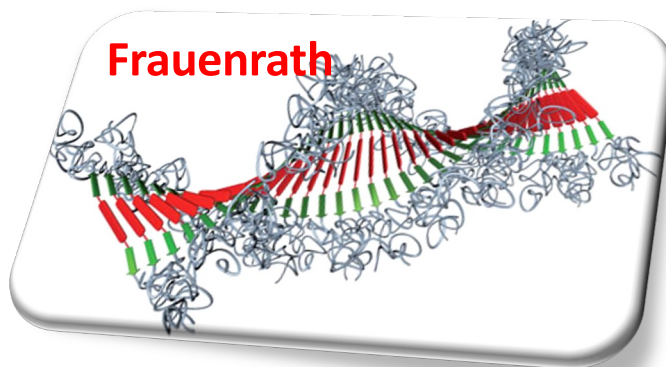
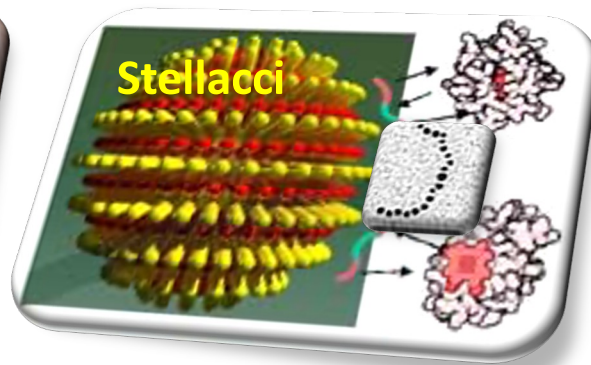
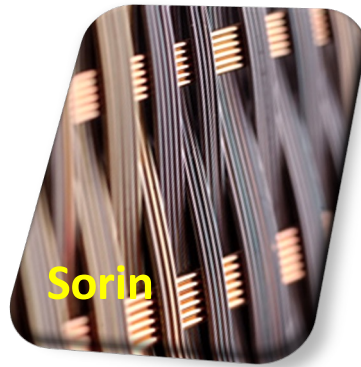
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Physical Origin of Material Properties



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Advanced materials' research

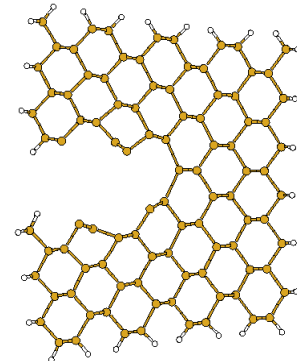
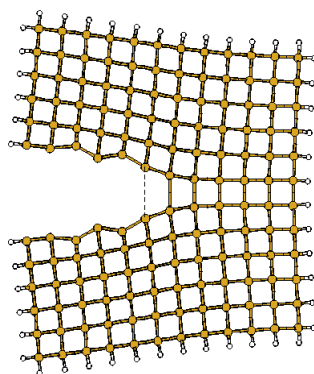
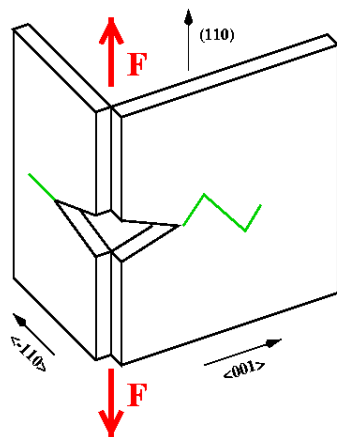


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Why do we need quantum mechanics ?

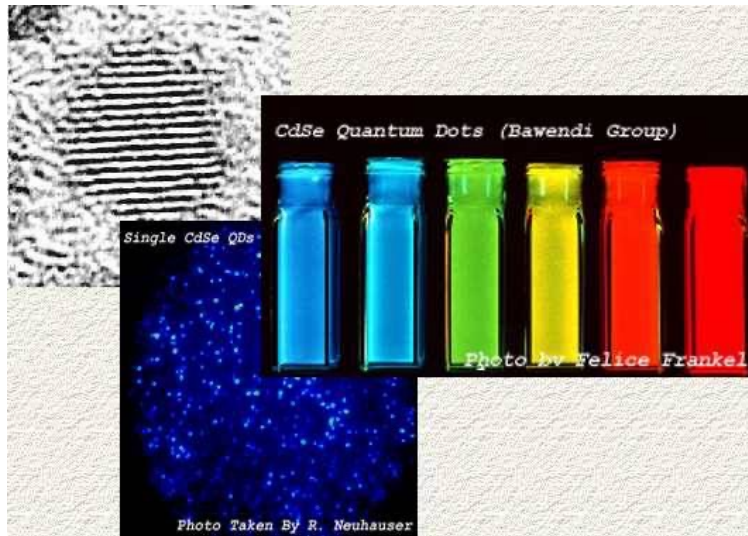
Structural properties (fracture in solids)



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Electronic, optical, magnetic properties



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Changing the world...

...for better or for worse

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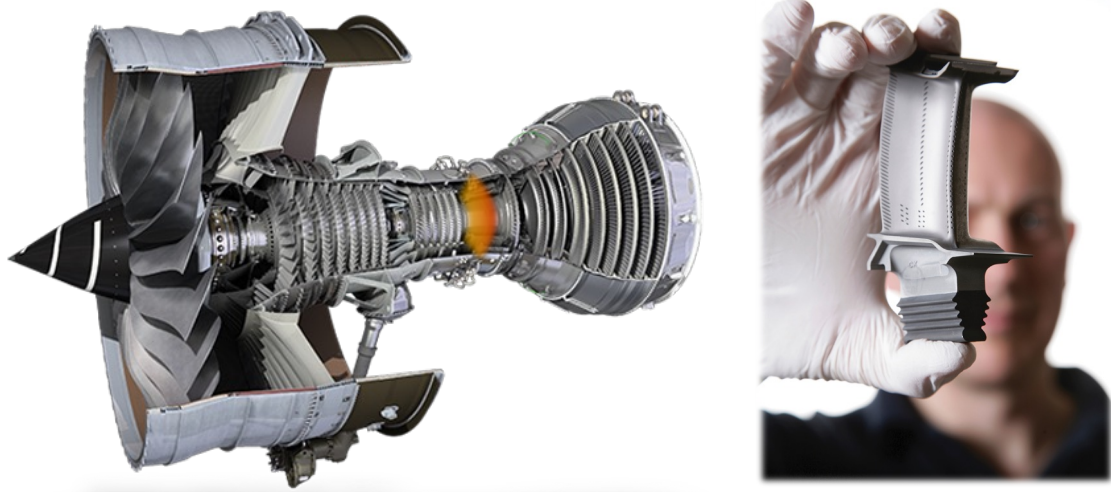
A few easy pieces



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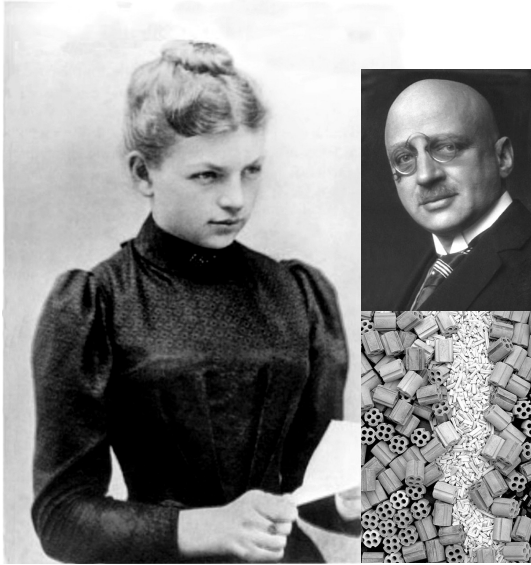
Next time you fly



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Meet Clara and Fritz

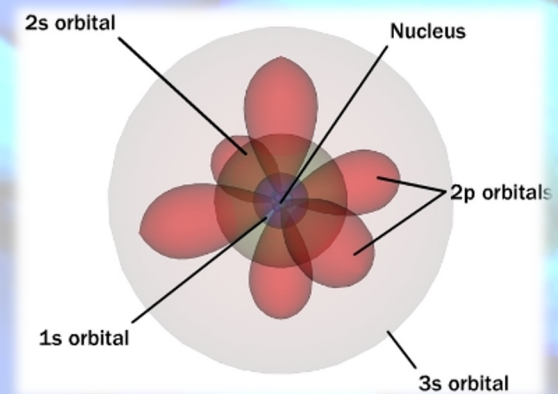


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Standard Model of Matter

- 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 = 1.602×10^{-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

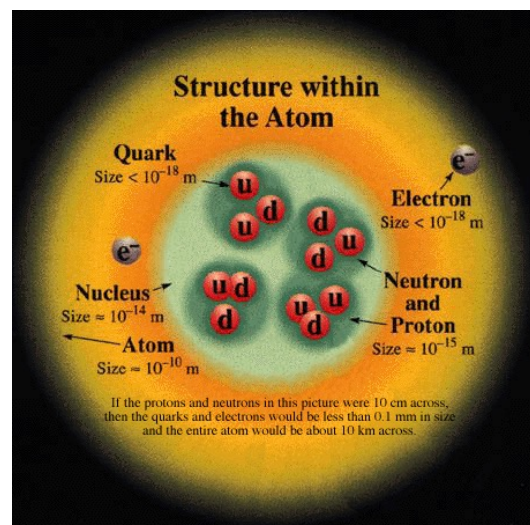
- Particles and electromagnetic fields
- Forces
- Dynamics

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Particles

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

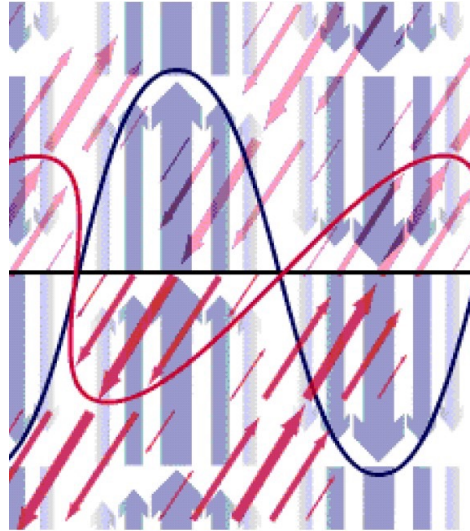


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Fields

- 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 = 6.626×10^{-34} J s

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

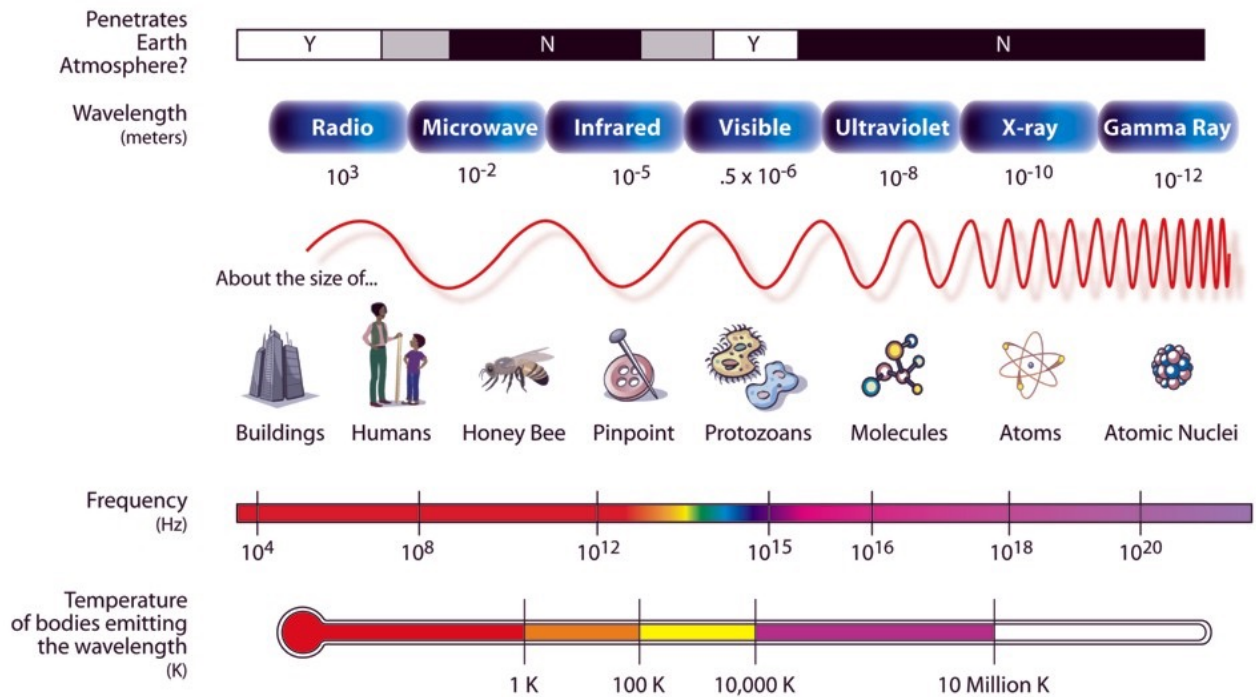
k is Boltzmann's constant = 1.381×10^{-23} J/K

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

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

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

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



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Dynamics of a Particle

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

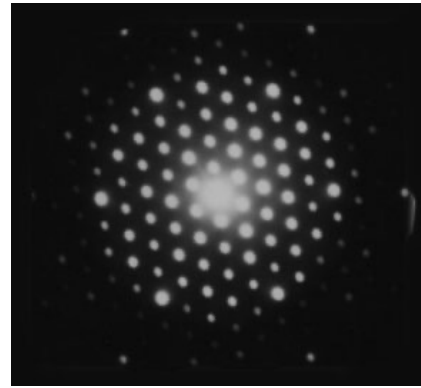
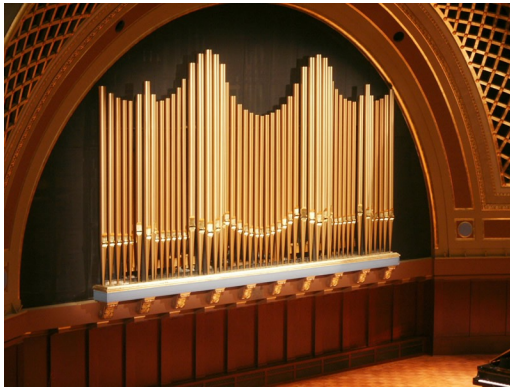
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Wave-particle Duality

- 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...)

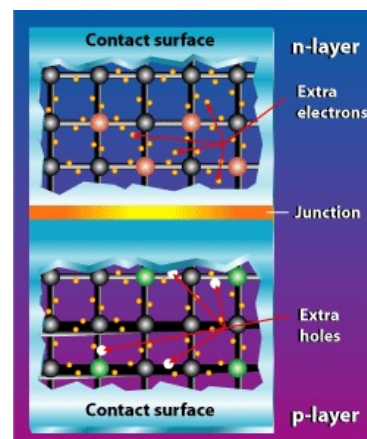
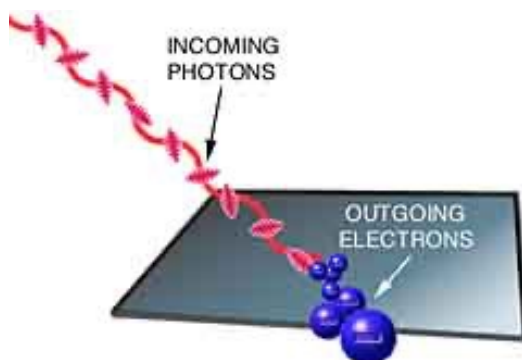


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Wave-particle Duality

- *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*

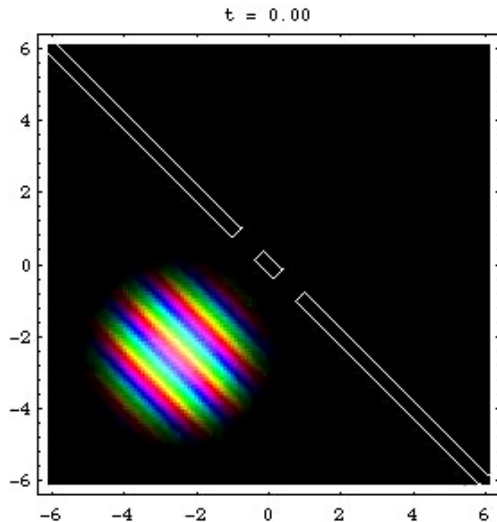


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When is a particle like a wave ?

Wavelength • momentum = Planck



$$\lambda \cdot p = h$$

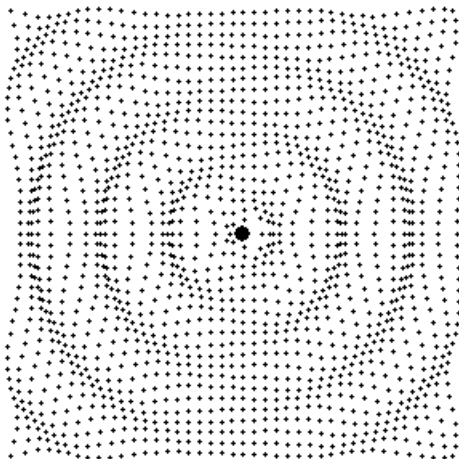
$$(h = 6.626 \times 10^{-34} \text{ J s} = 2\pi \text{ a.u.})$$

<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

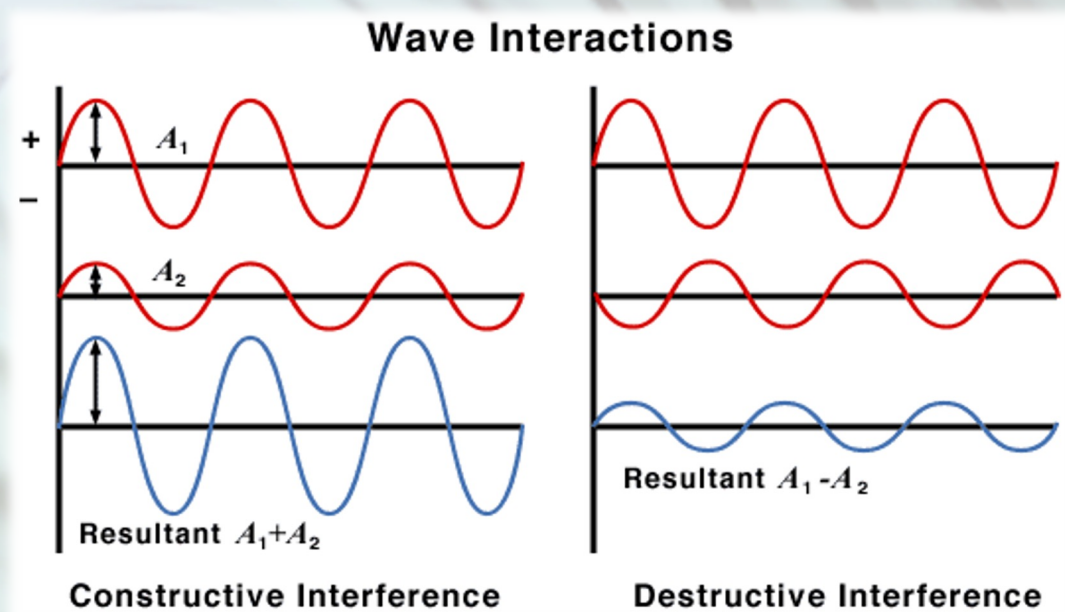
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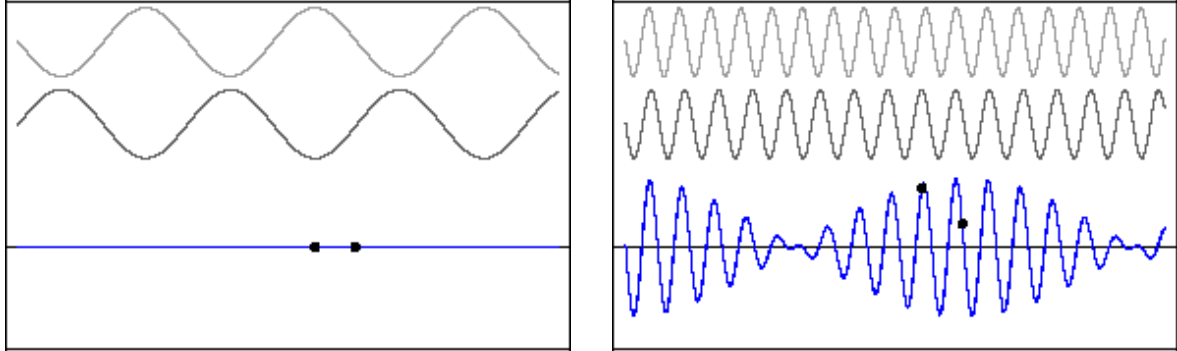
Principle of linear superposition



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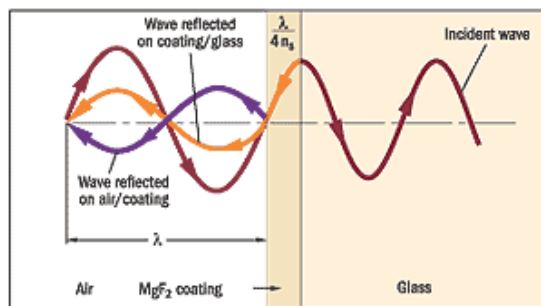
Interference in Action



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Interference in Action



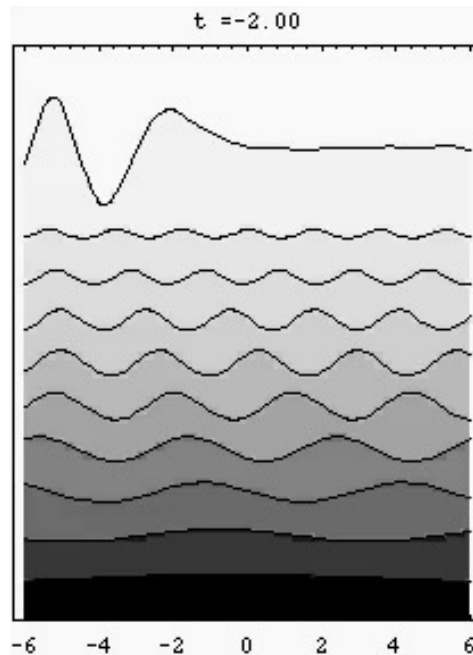
Source: Carl Zeiss Inc.



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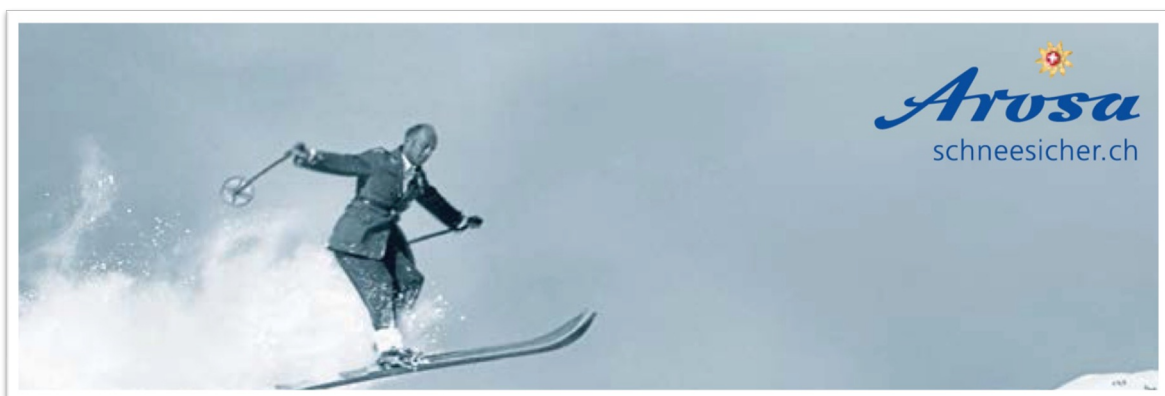
Also: decomposition of arbitrary functions into sines/cosines



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AROSA (GRAUBÜNDEN/GRISONS), 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

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Time-dependent Schrödinger's equation

(Newton's 2nd 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

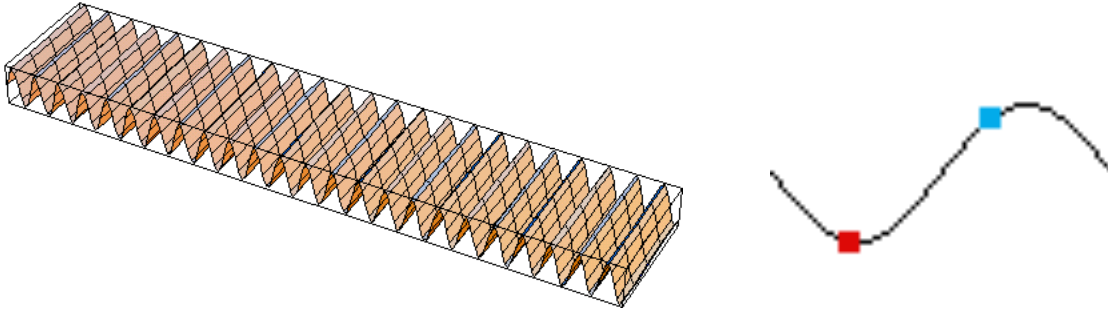
$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) = i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} \quad (\text{provided } E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m})$$

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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)

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

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