

# Introduction to matter –radiation interaction

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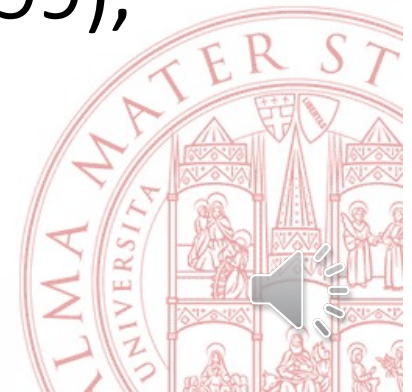
# Content

- Macroscopic
  - Dielectric response of matter
    - Index of refraction, dielectric function
    - Attenuation and dispersion
  - Model dielectric functions
- Microscopic
  - Phenomenology, from IR to x-rays
  - Cross section and attenuation coefficient
  - Scattering processes and the atomic form factor
  - Photoelectric absorption
    - absorption edges, de-excitation processes
- Relation between the atomic form factor and index of refraction
- Interaction between radiation and hydrogen – like atoms, semi-classical
  - Photoelectric absorption cross - section
  - Scattering cross - section



# References

- This presentation
- J.D. Jackson, *Classical Electrodynamics*, Wiley, 3rd Edition, 7.1, 7.2, 7.5 (parts)
- J. Als – Nielsen and D. McMorrow, *Introduction to Modern X-ray Physics*, Wiley, New York, 2001, Chap. 1
- D. Attwood, *Soft X-rays and extreme ultraviolet radiation*, Cambridge University Press (1999), Chapters 1 & 2



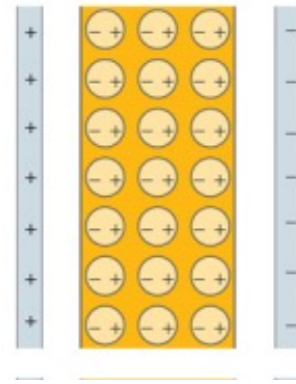
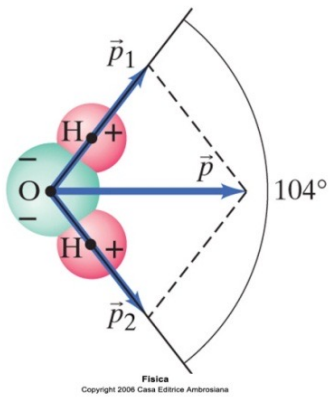
# Dielectric response

- General problem: how does condensed matter respond to the application of an external perturbation?
- The EM wave is the external perturbation
- First approach:  
macroscopic / collective
- Second approach:  
microscopic / atomic / particle



# Elementary phenomenology

- An electric field applied to a dielectric (no free charges) polarization
  - By distortion
  - By orientation



# Dielectric response

- The applied field will in general have a space and time dependence  $\vec{E}(\vec{r}, t)$  which will affect the response



# Polarization and susceptibility

- Assume the response of matter to the applied field is linear
  - OK for not too high fields
  - not OK for high power visible, EUV and X-ray lasers
- Apply linear response theory
- The electric dipole moment per unit volume is the polarization vector  $\vec{P}$
- Within the linear approximation introduce the electric susceptibility  $\chi$

$$\vec{P} = \varepsilon_0 \chi \vec{E}$$



# Polarization and susceptibility

- Susceptibility is in general a tensor quantity; for simplicity here consider it a scalar.
- We will study the scalar relations in the frequency domain

$$P(\omega) = \varepsilon_0 \chi(\omega) E(\omega)$$

- The dielectric response of matter determines  $\chi(\omega)$





# Dielectric displacement

- The dielectric displacement vector is defined as

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P}$$

- The direct proportionality between  $\vec{D}$  and  $\vec{E}$  is written as

$$\vec{D} = \varepsilon_0 \varepsilon \vec{E}$$

in which  $\varepsilon$  is the «dielectric constant», better called permittivity or dielectric function

- Clearly

$$\varepsilon = 1 + \chi$$



# Dielectric displacement

- We will study dynamics (time dependent properties)
- Susceptibility and dielectric function are «linear response functions»
  - Independent of the external field
  - Describe system properties



# The dielectric function

- $D(\omega) = \varepsilon_0 \varepsilon(\omega) E(\omega)$ 
  - $\varepsilon(\omega)$  has a real and imaginary part:  $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$
- The  $\omega$  dependence of  $\varepsilon$  is determined by
  - The spectral range
  - The corresponding type of excitations possible
  - The specific properties of the system

Spectral range	System	Excitation processes
Micro - waves	Molecules, free or in solution	Molecular rotations
Infra - red	Molecules, free or in solution	Molecular vibrations
Infra - red	Solids	Phonons
Visible – UV	Atoms, molecules, solids	Valence electron transitions
X - rays	Atoms, molecules, solids	Core level electron transitions



# Dispersion and attenuation

- The dielectric function determines dispersion and attenuation of an EM wave propagating in a polarizable medium
  - a not too rarefied gas, a liquid, a solid or any other state of aggregation (liquid crystal, plasma ...)
- In vacuum the dispersion relation for EM waves is

$$\omega = ck$$

$c$  is the speed of light in vacuo.



# Dispersion and attenuation

- In the medium the dispersion relation is modified by the presence of the index of refraction  $n(\omega)$ :

$$\omega = \frac{c}{n(\omega)}k$$

- The index of refraction is

$$n(\omega) = \sqrt{\varepsilon(\omega)\mu(\omega)}$$

- Neglecting magnetic effects,  $\mu(\omega) = 1$

$$n(\omega) = \sqrt{\varepsilon(\omega)}$$

- $n(\omega)$  and  $\varepsilon(\omega)$  are macroscopic quantities which describe the interaction between the wave and the medium



# Dispersion and attenuation

- Consider a plane wave propagating along  $x$

$$E = E_0 e^{i(kx - \omega t)}; \quad k(\omega) = \frac{n(\omega) \omega}{c}$$

- $n(\omega)$  has a real and an imaginary part:

$$n(\omega) = n_1(\omega) + i n_2(\omega)$$

- Therefore, also the wave number has a real and imaginary part

$$k(\omega) = \frac{[n_1(\omega) + i n_2(\omega)] \omega}{c} = k_1(\omega) + i k_2(\omega)$$

$$k_1(\omega) = \frac{n_1(\omega) \omega}{c}, \quad k_2(\omega) = \frac{n_2(\omega) \omega}{c}$$



# Dispersion and attenuation

- $k(\omega) = \frac{[n_1(\omega) + in_2(\omega)] \omega}{c} = k_1(\omega) + ik_2(\omega)$   
 $k_1(\omega) = \frac{n_1(\omega) \omega}{c}, k_2(\omega) = \frac{n_2(\omega) \omega}{c}$
- The effect on the space propagation is

$$e^{ikx} = \underbrace{e^{ik_1(\omega)x}}_{\text{Propagation term}} \underbrace{e^{-k_2(\omega)x}}_{\text{Attenuation term}}$$

Propagation term

Attenuation term

- The space – time dependence of the wave is thus

$$E = E_0 e^{i[k_1(\omega)x - \omega t]} e^{-k_2(\omega)x}$$



# Dispersion and attenuation

- $E = E_0 e^{i[k_1(\omega)x - \omega t]} e^{-k_2(\omega)x}$
- $k_1(\omega) = \frac{\omega n_1(\omega)}{c}$  is the modified wave vector
  - the phase velocity of the wave is  $v = \frac{c}{n_1(\omega)}$
- $k_2(\omega) = \frac{\omega n_2(\omega)}{c}$  determines the attenuation of the wave as it traverses the medium
- $n_1(\omega)$ : dispersion (modifies the speed of propagation)
  - If the wave crosses the interface between two media it will change direction (refraction)
- $n_2(\omega)$ : attenuation





# The linear attenuation coefficient

- $k_2(\omega) = \frac{\omega n_2(\omega)}{c}$ : attenuation of the amplitude
- Since  $I \propto |E|^2$  the attenuation coefficient of the intensity is

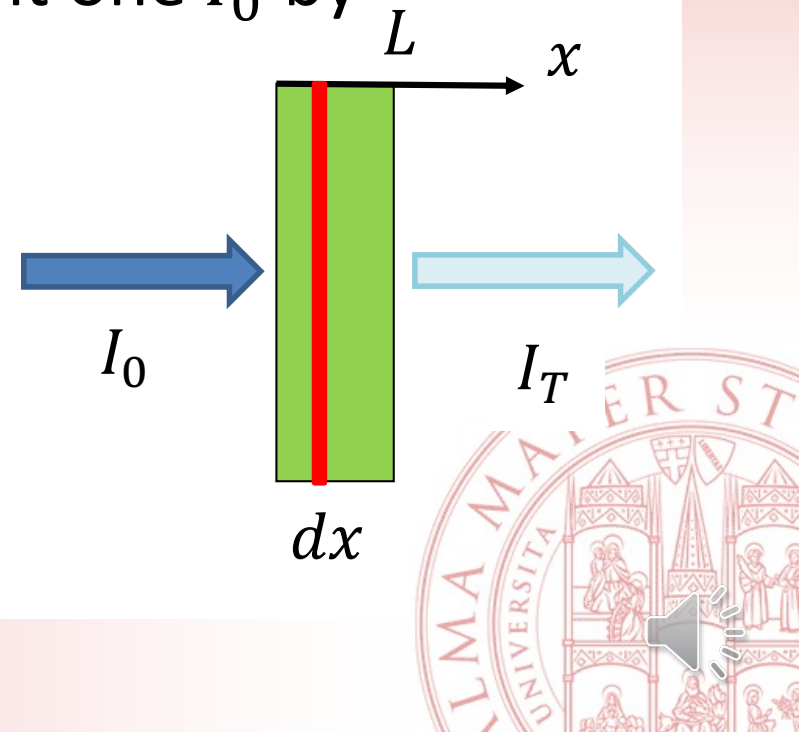
$$\mu = \frac{2\omega n_2(\omega)}{c}$$

- If the total thickness traversed is  $L$  the transmitted intensity  $I_T$  is related to the incident one  $I_0$  by

$$I_T = I_0 e^{-\mu L}$$

- For an infinitesimal thickness

$$\frac{dI}{I} = -\mu dx$$



# Relation between $\varepsilon(\omega)$ e $n(\omega)$

- $n_1(\omega) + in_2(\omega) = \sqrt{\varepsilon_1(\omega) + i\varepsilon_2(\omega)}$
- Therefore:
  - $\varepsilon_1 = n_1^2 - n_2^2$ ,  $\varepsilon_2 = 2n_1n_2$
  - $n_1 = \frac{\sqrt{\varepsilon_1 + |\varepsilon|}}{\sqrt{2}}$ ,  $n_2 = \frac{\sqrt{-\varepsilon_1 + |\varepsilon|}}{\sqrt{2}}$



## Relation between $\varepsilon(\omega)$ e $n(\omega)$ – weak interaction

- With  $\varepsilon = 1 + \varepsilon' + i\varepsilon_2$  if  $\varepsilon'$  and  $\varepsilon_2 \ll 1$ :  
weak interaction limit (X-ray range)

- In this limit

$$n = \sqrt{1 + \varepsilon' + i\varepsilon_2} \cong 1 + \frac{1}{2}\varepsilon' + i\frac{1}{2}\varepsilon_2$$

- By convention, in the weak interaction limit the index of refraction is written as

$$n(\omega) = 1 - \delta(\omega) + i\beta(\omega)$$

$$\delta = -\frac{1}{2}\varepsilon', \quad \beta = \frac{1}{2}\varepsilon_2$$

$$\delta \text{ and } \beta \ll 1$$



# Model dielectric functions

- Study two simple models for  $\varepsilon(\omega)$  to illustrate general features of the dielectric response of matter
  - Static ( $\omega = 0$ ) distortion polarization
  - Damped harmonic oscillator



# Static distortion polarization

- A static electric field applied to a classical molecule consisting of point charges: nuclei and electrons
- $N$  charges  $q_j$  with mass  $m_j$ , elastically bound to their equilibrium position by a restoring force

$$-m_j \omega_j^2 r_j$$

in which  $r_j$  is the displacement of the  $j$ -th charge in the direction of the electric field

- $j = 1, \dots, N$
- $\omega_j$  is the resonance frequency of the  $j$ -th charge



# Static distortion polarization

- The force acting on each charge is  $q_j E$
- At equilibrium the displacement of each charge is

$$r_j^e = \frac{q_j}{m_j \omega_j^2} E$$

- The induced dipole moment is  $p_j = \frac{q_j^2}{m_j \omega_j^2} E$
- The total induced dipole moment is

$$\sum_{j=1}^N \frac{q_j^2}{m_j \omega_j^2} E$$



# Static distortion polarization

- If the (number) density of molecules is  $\rho$  the static permittivity is

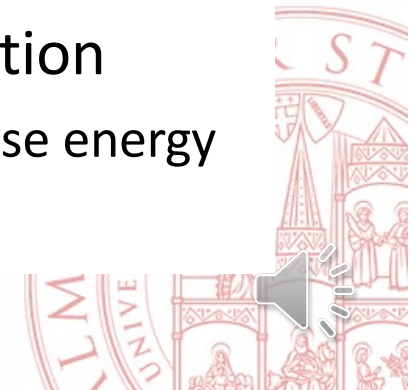
$$\varepsilon(\omega = 0) = 1 + \frac{\rho}{\varepsilon_0} \sum_{j=1}^N \frac{q_j^2}{m_j \omega_j^2}$$

- Always  $> 1$
- Reasonable behaviour as a function of masses, density and resonance frequency
  - increases with  $\rho$
  - decreases with  $m_j$  and  $\omega_j$



# Damped harmonic oscillator: approximations

- In describing the effect of an EM on a collection of charges which simulate the dielectric response of matter we make the following important approximations
  - 1) Electric dipole approximation
    - $\lambda \gg$  displacement of charges (neglect spatial variation of field): validity depends on spectral range
  - 2) Neglect motion of nuclei, consider only the contribution of electrons
    - Justified in view of the great difference in mass
  - 3) Neglect effect of force  $q(\vec{v} \times \vec{B})$  due to magnetic field
    - Justified since it is weaker than  $qE$
  - 4) Neglect «radiation damping» due to emission of radiation
    - An accelerated charge will always emit radiation: it will thus lose energy
    - This effect is often considered as due to a «self – force».





# Damped harmonic oscillator

- First consider a single electron
  - equilibrium position in the origin, displacement  $r$  at time  $t$
  - charge  $-e$  and mass  $m$
  - elastically bound to its equilibrium position by a restoring force

$$-m\omega_0^2 r$$

➤  $\omega_0$  is the resonant frequency (frequency of unforced oscillations)

- subject to a dissipative viscous force

$$-m\gamma \frac{dr}{dt}$$



# Damped harmonic oscillator

- The external electric field is written as

$$E_0 e^{-i\omega t}$$

- The classical equation of motion is

$$-eE_0 e^{-i\omega t} - m\omega_0^2 r - m\gamma \frac{dr}{dt} = m \frac{d^2 r}{dt^2}$$



# Damped harmonic oscillator

- We seek a solution of the type  $r(t) = R(\omega)e^{-i\omega t}$
- We easily find

$$R(\omega) = \frac{e}{m(\omega^2 - \omega_0^2 + i\gamma\omega)} E_0$$

- The induced dipole moment is

$$p(\omega)e^{-i\omega t} = \frac{e^2}{m(\omega_0^2 - \omega^2 - i\gamma\omega)} E_0 e^{-i\omega t}$$



# An atom as an ensemble of oscillators

- Model an atom as composed of  $Z$  electrons arranged in  $M$  shells with equal characteristic  $\omega_j, \gamma_j$

- Each shell contains  $f_j$  electrons, with

$$\sum_{j=1}^M f_j = Z$$



# An atom as an ensemble of oscillators

- Following the single electron result, the atomic dipole moment induced by the external field is

$$p(\omega) = \frac{e^2}{m} \sum_{j=1}^M \frac{f_j}{(\omega_j^2 - \omega^2 - i\gamma_j\omega)} E_0$$

- $f_j$  is known as the «oscillator strength»: it determines the contribution of the  $j$ -th shell to the dipole moment



## A medium as an ensemble of polarizable atoms

- If the (number) density of identical atoms is  $\rho$ , we find

$$\varepsilon(\omega) = 1 + \frac{\rho e^2}{\varepsilon_0 m} \sum_{j=1}^M \frac{f_j}{(\omega_j^2 - \omega^2 - i\gamma_j \omega)}$$

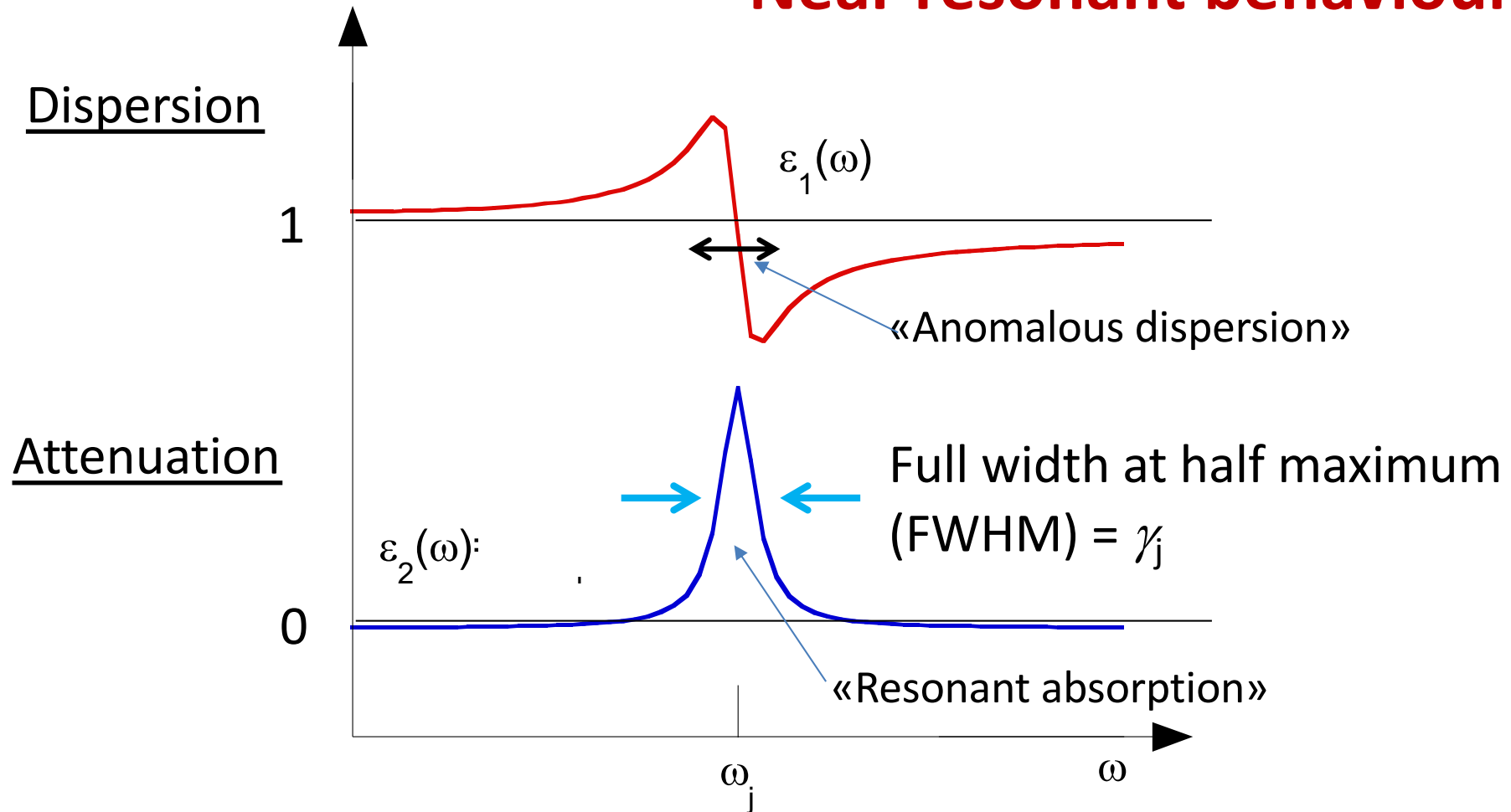
- $\varepsilon_1(\omega) = 1 + \frac{\rho e^2}{\varepsilon_0 m} \sum_{j=1}^M \frac{f_j(\omega_j^2 - \omega^2)}{[(\omega_j^2 - \omega^2)^2 + (\gamma_j \omega)^2]}$

- $\varepsilon_2(\omega) = \frac{\rho e^2}{\varepsilon_0 m} \sum_{j=1}^M \frac{f_j \gamma_j \omega}{[(\omega_j^2 - \omega^2)^2 + (\gamma_j \omega)^2]}$

- Kramers – Heisenberg or electric dipole dielectric function



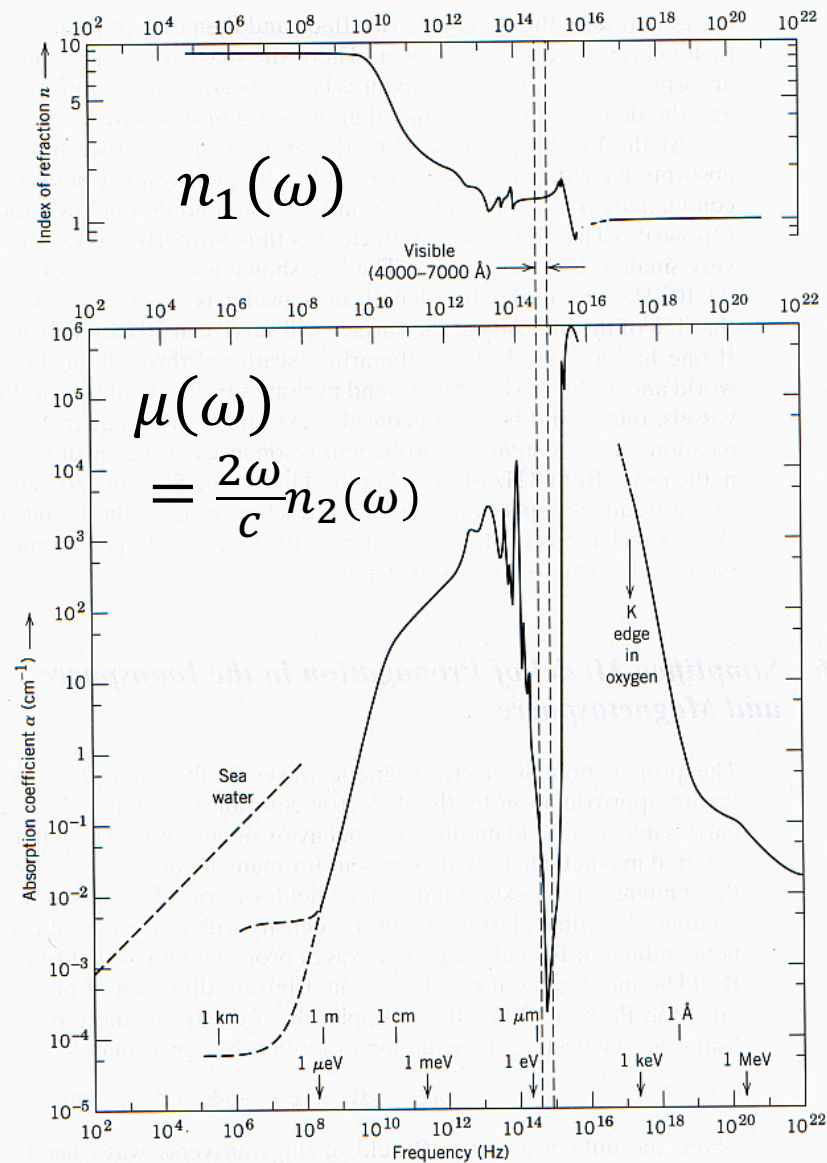
# Near resonant behaviour



- A simple model which reproduces well the response of polarizable media in many frequency ranges



# The dielectric response of liquid water as a function of frequency



**Figure 7.9** The index of refraction (top) and absorption coefficient (bottom) for liquid water as a function of linear frequency. Also shown as abscissas are an energy scale (arrows) and a wavelength scale (vertical lines). The visible region of the frequency spectrum is indicated by the vertical dashed lines. The absorption coefficient for seawater is indicated by the dashed diagonal line at the left. Note that the scales are logarithmic in both directions.

