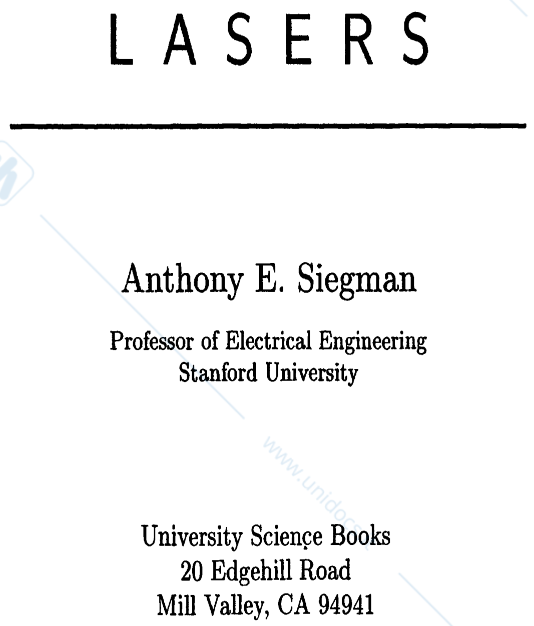
PART B- Optical properties of semiconductors

LESSON B1-
The classical electron oscillator model

Reference



LASERS

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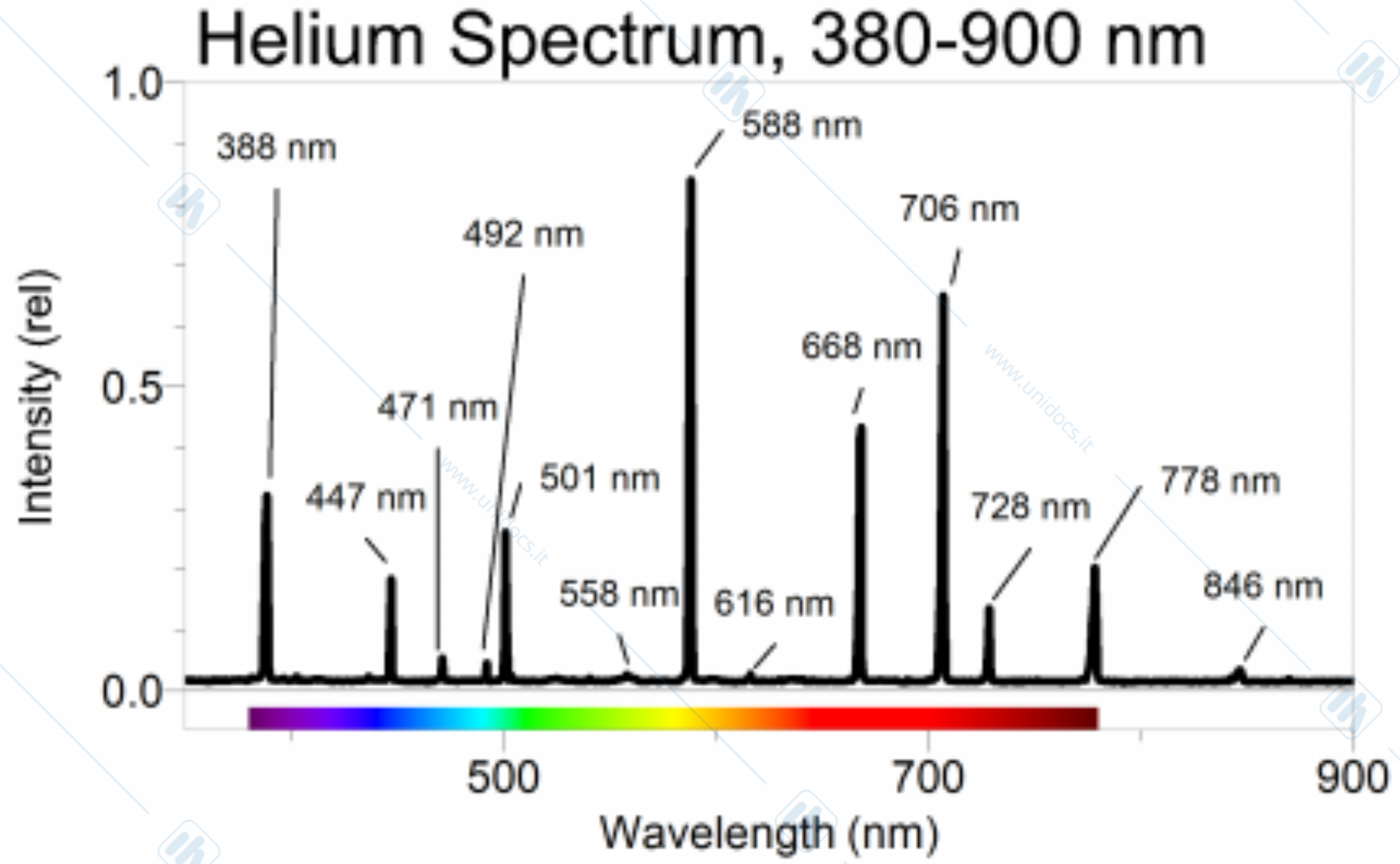
Chapter 2 and chapter 4

Spontaneous emission of light

- **Spontaneous emission** is the process in which a quantum mechanical system (such as an atom, molecule or subatomic particle) transitions from an excited energy state to a lower energy state (e.g., its ground state) and emits a quantum in the form of a photon. Spontaneous emission is ultimately responsible for most of the light we see all around us.

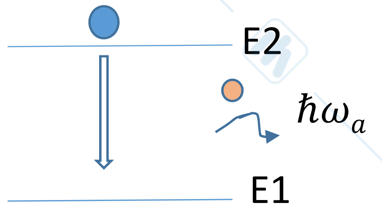
https://en.wikipedia.org/wiki/Spontaneous_emission

Spontaneous emission from atoms

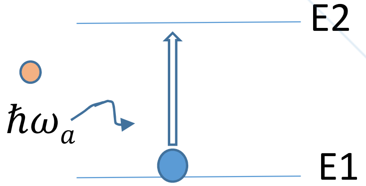


Spontaneous/ stimulated emission of light

and absorption of light

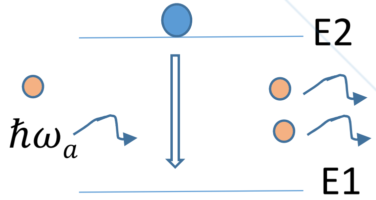


Spontaneous emission



Absorption

Light absorption



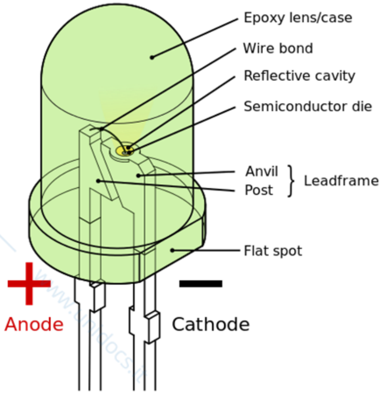
Stimulated emission

Light
amplification

In semiconductor devices …

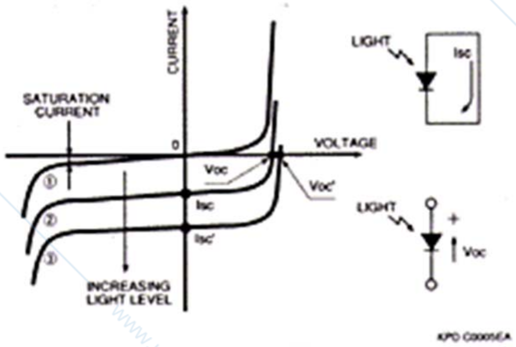
Spontaneous emission of light

LEDs

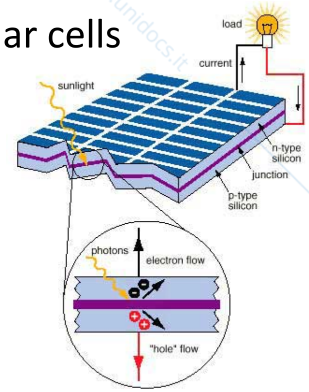


Absorption of light

Photodiodes and solar cells

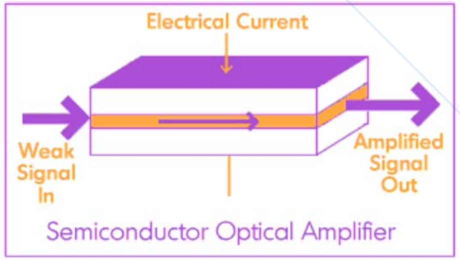


Solar cells

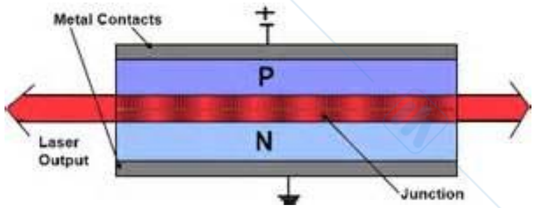


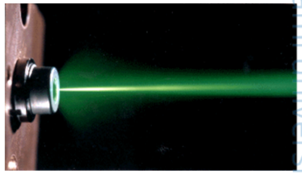
Stimulated emission of light

Semiconductor optical amplifiers



Laser diodes





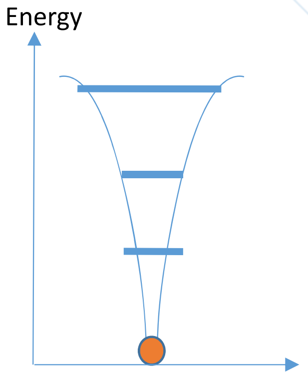
The classical oscillator model

- Goal: understand how optical signals act on atoms (or ions, or molecules) to excite resonance response and to cause transitions between atomic energy levels.

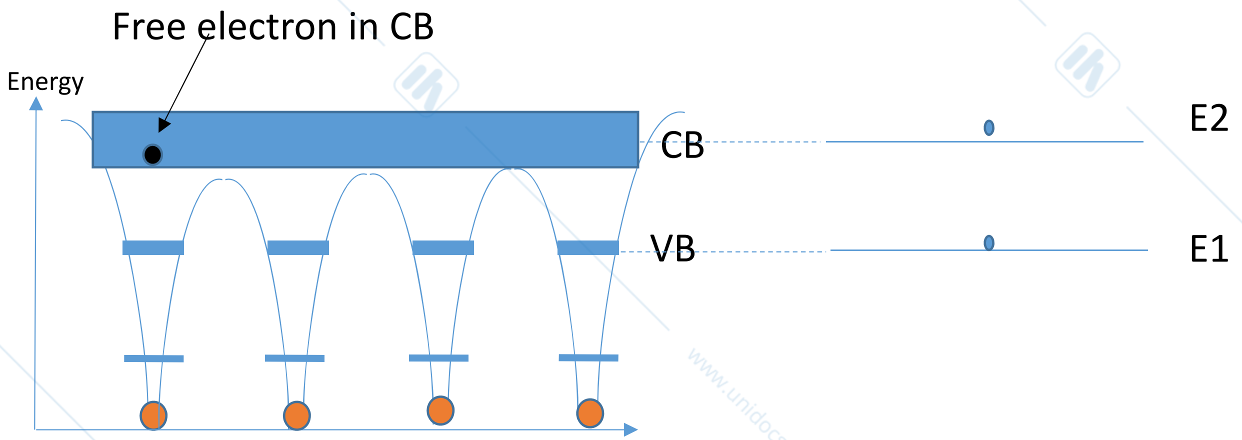
- The term “atoms” is generally used as a shorthand for ions, or molecules in solids or liquids, or even for valence band and conduction band electrons responsible for optical transitions in semiconductors.

Reference: Siegman, “Lasers”, Ed. University Science book, chapter 2

Valence band and conduction band in semiconductor



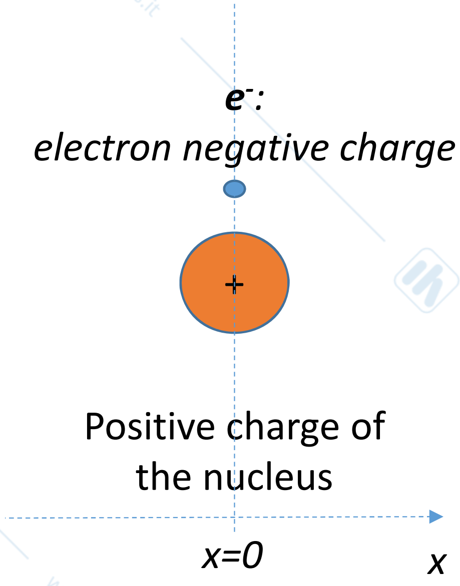
Electron energy levels of a single atom



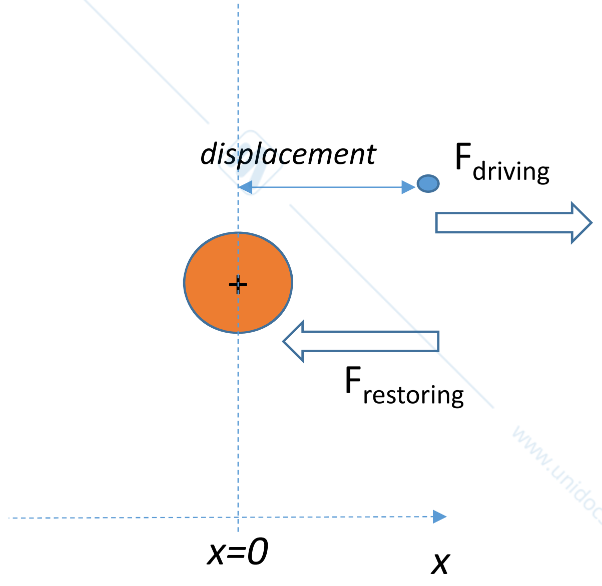
Energy bands in semiconductor

We will use the classical oscillator model to understand how the optical signals acts on the electrons in state E1 (=electron in VB) or state E2 (=electron in CB). We will learn that the electric field can promote a transition from E1 to E2.

Classical electron oscillator model

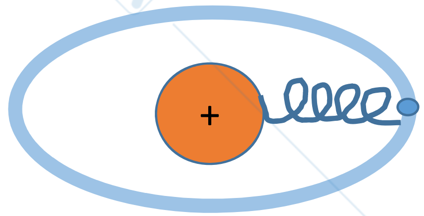


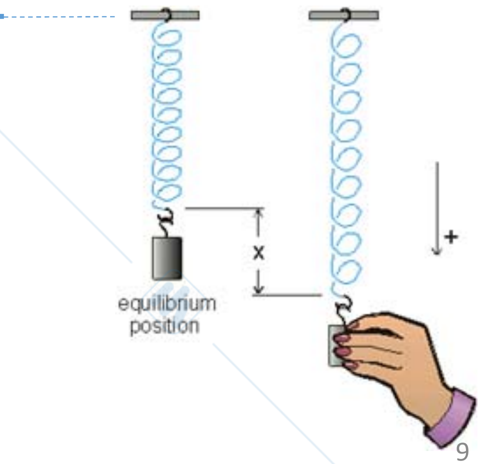
Equilibrium



Displacement from equilibrium

Equivalent spring-mass system





$F_{driving}$=$-e \cdot E_x(t)$: externally applied signal with electric field $E_x(t)$

$F_{restoring}$=$-K \cdot x(t)$: due to the positive charge of the nucleus, the electron experiences a linear restoring force

Analysis: goals

- We want understanding:

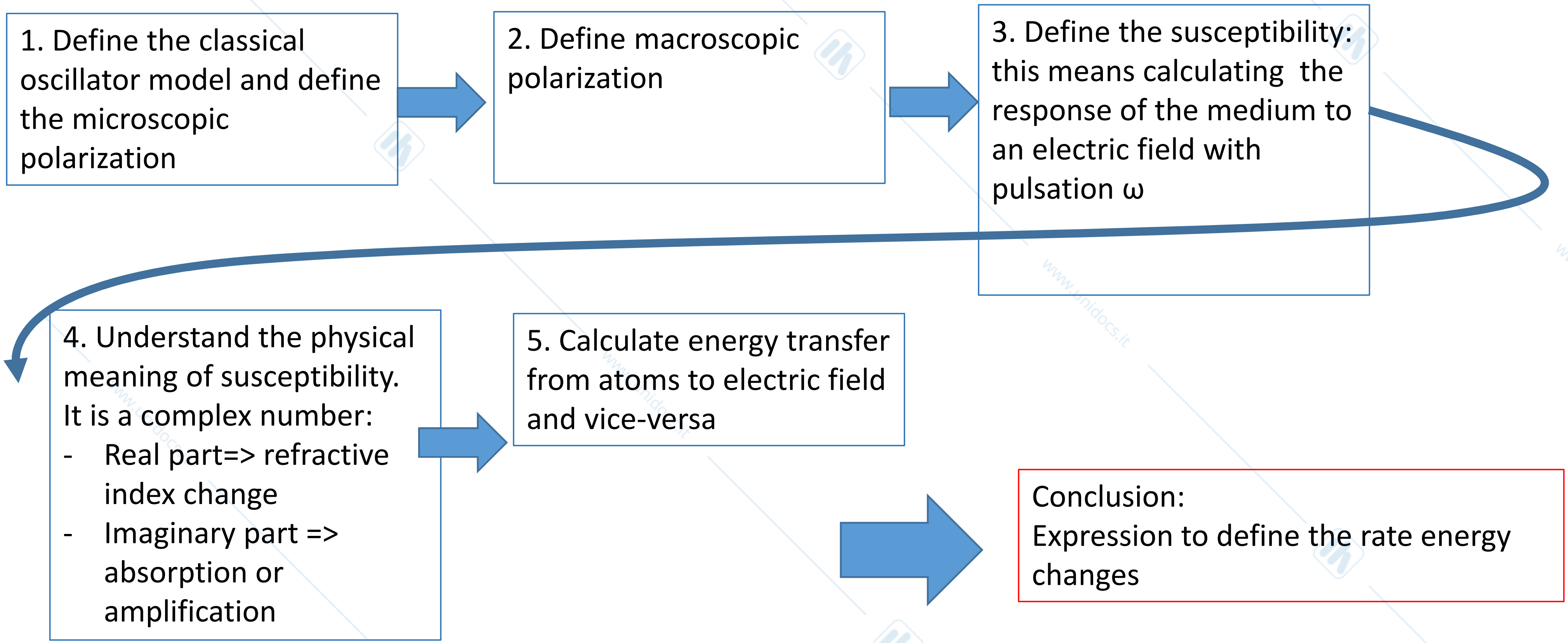
  - how the applied electric field modifies the microscopic dipole

  - how this impact macroscopic polarization

  - how the electric field transfers energy to the atoms and vice-versa

- As a result of this analysis we will define Absorption (ie: how much energy is transferred from the electric field to the atoms) and Amplificariron (ie: how much energy is transferred from atoms to the electric field) coefficients

Analysis: summary of main steps



1. Define the classical oscillator model and define the microscopic polarization

2. Define macroscopic polarization

3. Define the susceptibility: this means calculating the response of the medium to an electric field with pulsation ω

4. Understand the physical meaning of susceptibility. It is a complex number:
- Real part=> refractive index change
- Imaginary part => absorption or amplification

5. Calculate energy transfer from atoms to electric field and vice-versa

Conclusion:
Expression to define the rate energy changes

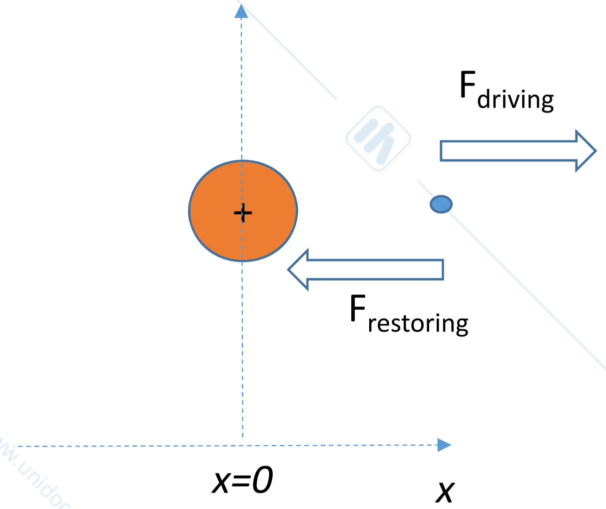
Analysis: Calculate x(t) depending on Ex(t)

mass

$$m\frac{d^2x(t)}{dt^2} = F_{tot} = F_{driving} + F_{restoring}$$

Elastic constant

$$m\frac{d^2x(t)}{dt^2} = -k_0x(t) - e\mathcal{E}_x(t)$$



Displacement from equilibrium

Let’s consider first the case with no driving force:

$$\frac{d^2x(t)}{dt^2} + \frac{k_0}{m}x(t) = 0 \qquad \omega_a^2 = \frac{k_0}{m}$$

ω_a is the classical oscillator resonance frequency

Damping

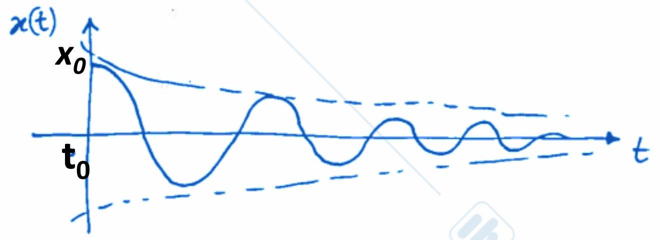
The oscillation of the electron around the equilibrium position is damped for several physical reasons. The electron will loose energy with time and return to the equilibrium position when the driving force is suspended. **We add the damping term** in the equation of motion:

$$\frac{d^2x(t)}{dt^2} + \gamma\frac{dx(t)}{dt} + \omega_a^2 x(t) = -\frac{e}{m}\mathcal{E}_x(t)$$

$$x(t) = x(0)e^{-\frac{\gamma}{2}t} \cdot e^{j\omega_a' t}$$

$$\omega_a' = \sqrt{\omega_a^2 - \left(\frac{\gamma}{2}\right)^2} \simeq \omega_a$$

Let’s move the electron in x(0)=x_0 at t=t_0 by using an applied electric field; then we remove the field at t>t_0. The electron returns in the equilibrium position with damped relaxation oscillations



Energy and spontaneous decay

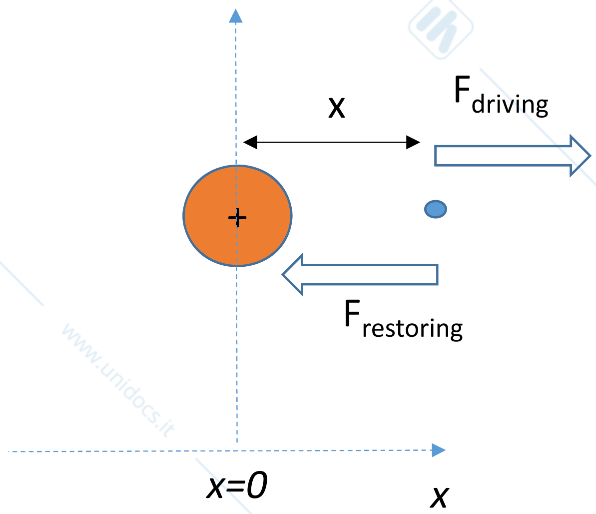
Energy associated with the internal oscillation:

$$U_a(t) = k_0 x^2(t) + \frac{1}{2} m v_x^2(t) = U(0) e^{-\gamma t}$$

- We see that energy decays at a rate determined by γ. The decay rate (γ) is thus the energy decay rate
- Energy is lost in part by radiating away electromagnetic radiation (spontaneous emission or fluorescence) at the resonance frequency w_a
- Other non radiative mechanism are however possible (collision with other atoms or heat emission) => non-radiative energy loss

Microscopic dipole moment

- The displacement of the electron respect to the nucleus means that there is a displacement of the negative charge respect to the positive one.
- This displacement creates a microscopic electric dipole moment



Displacement from equilibrium

$$\mu_x(t) = [charge] \times [displacement] = -ex(t)$$

Equation of motion for any single microscopic dielectric dipole

$$\boxed{\frac{d^2\mu_x(t)}{dt^2} + \gamma\frac{d\mu_x(t)}{dt} + \omega_a^2\mu_x(t) = (e^2/m)\mathcal{E}_x(t)}$$

$$\mu_x(t) = \mu_{x0}\, e^{[-(\gamma/2)(t-t_0)+j\omega_a(t-t_0)+j\phi_0]}$$

Macroscopic polarization

- The macroscopic polarization is then calculated by averaging the microscopic dipole moments.

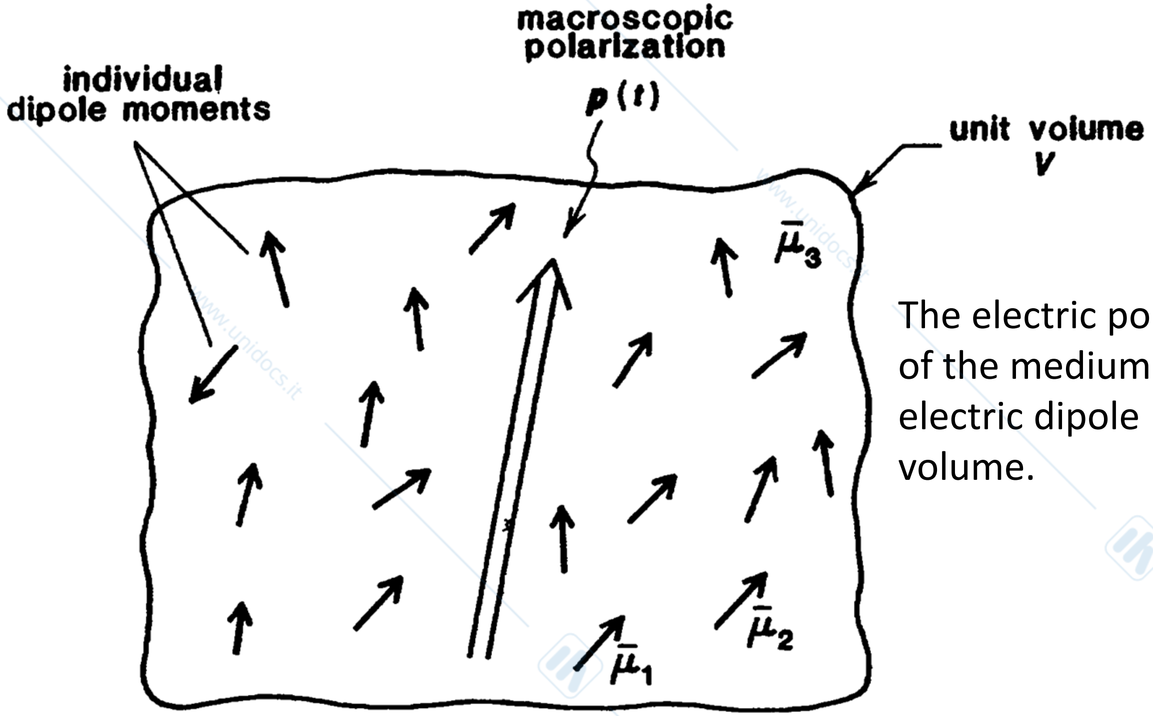


FIGURE 2.4
Macroscopic electric polarization produced by a collection of individual dipole moments.

The electric polarization at any point of the medium is by definition the net electric dipole moment per unit of volume.

Macroscopic polarization: equations

Let each atom in this volume be labeled by an index i, and let each atom have an instantaneous electric dipole moment $\mu_{xi}(t) = -ex_i(t)$.

This medium will then have a macroscopic electric polarization $\boldsymbol{p}$ around that point $\boldsymbol{r}$ in the medium whose x component is given by

$$p_x(\boldsymbol{r}, t) \equiv V^{-1} \sum_{i=1}^{NV} \mu_{xi}(t).$$

Because we assume that the electric field is applied in the *x* direction (ie: E_x(t))

Macroscopic polarization: equations

- Let’s consider first the simple case when all dipoles are oscillating in phase

$$\mu_{x,\mathrm{tot}}(t) = \sum_{i=1}^{NV} \mu_{x,i}(t) = NV\mu_x(t) \qquad \left\{\begin{array}{l}\text{all dipoles}\\ \text{oscillating}\\ \text{in phase,}\end{array}\right.$$

$$p_x(t) = N\mu_{x0}\, \exp[[-(\gamma/2) + j\omega_a](t - t_0) + j\phi_0] \qquad \left\{\begin{array}{l}\text{all dipoles}\\ \text{oscillating}\\ \text{in phase.}\end{array}\right.$$

Polarization dephasing:
not all the dipoles
are in phase

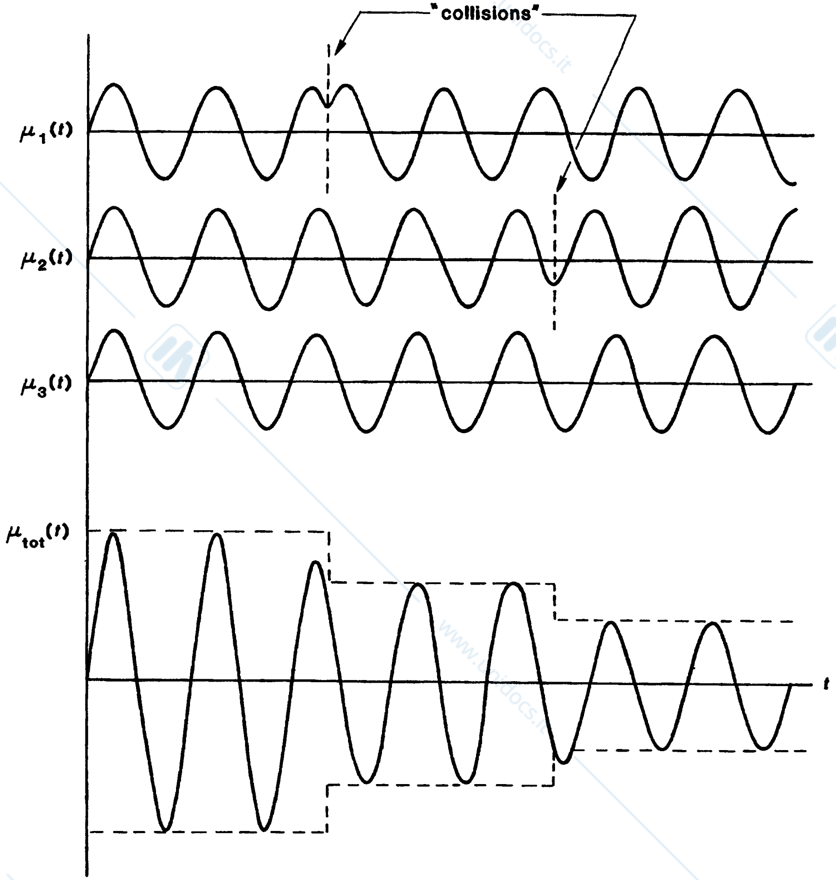


FIGURE 2.5
Decay of the total dipole moment resulting from random dephasing collisions in a collection of oscillating dipoles.

$$= p_{x0} \exp\left[-(\gamma/2 + 1/T_2)(t - t_0) + j\omega_a(t - t_0) + j\phi_0\right].$$

Summary slide

The primary conclusion of this section, therefore, is that although the macroscopic polarization $p_x(t)$, has the same resonance frequency as the individual microscopic dipole oscillations $\mu_x(t)$, it may have a faster decay rate because of dephasing effects. Individual atomic dipole oscillations, in the intervals between dephasing events, can thus be described as obeying the equation of motion

$$\frac{d^2\mu_x(t)}{dt^2} + \gamma\frac{d\mu_x(t)}{dt} + \omega_a^2\mu_x(t) = (e^2/m)\mathcal{E}_x(t)$$

with an amplitude decay rate $\gamma/2$. But the coherent polarization $p_x(t)$ must be described as obeying the equation

$$\frac{d^2p_x(t)}{dt^2} + (\gamma + 2/T_2)\frac{dp_x(t)}{dt} + \omega_a^2 p_x(t) = (Ne^2/m)\mathcal{E}_x(t),$$

where there is an additional factor of $1/T_2$ in the amplitude decay rate because the dephasing processes cause the oscillations of individual atoms to become randomized in phase at a rate $1/T_2$.

Polarization and Maxwell equations

The response of a medium to an electromagnetic field generates the *polarization* and the *magnetization*:

polarization (electric polarization)	$\boldsymbol{P}(\mathbf{r}, t)$	$\mathrm{C\,m^{-2}}$,
magnetization (magnetic polarization)	$\boldsymbol{M}(\mathbf{r}, t)$	$\mathrm{A\,m^{-1}}$.

They are connected to the field quantities through the following relations:

$$\boldsymbol{D}(\mathbf{r}, t) = \epsilon_0 \boldsymbol{E}(\mathbf{r}, t) + \boldsymbol{P}(\mathbf{r}, t)$$

and

$$\boldsymbol{B}(\mathbf{r}, t) = \mu_0 \boldsymbol{H}(\mathbf{r}, t) + \mu_0 \boldsymbol{M}(\mathbf{r}, t),$$

where

$$\epsilon_0 \approx \frac{1}{36\pi} \times 10^{-9}\ \mathrm{F\,m^{-1}}\ \text{or}\ \mathrm{A\,s\,V^{-1}\,m^{-1}}$$

Macroscopic electromagnetic effects

- Next important step is to go **from the microscopic individual atoms** (represented by the individual electron oscillators) **to macroscopic electromagnetic effects** in real semiconductor materials.

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\nabla \times \boldsymbol{H} = \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t}$$

Calculation of the macroscopic polarization

$$\mathcal{E}_x(t) = \mathrm{Re}\left\{\tilde{E}_x\, e^{jwt}\right\} = \frac{1}{2}\left[\tilde{E}_x\, e^{jwt} + \tilde{E}_x^*\, e^{-jwt}\right]$$

We apply an Electric field with pulsation **ω** to a collection of atoms

$$P_x(t) = \frac{1}{2}\left[\tilde{P}_x\, e^{jwt} + \tilde{P}_x^*\, e^{-jwt}\right]$$

We want calculating how the response of the medium depends on the pulsation **ω** ; ie: we calculate the macroscopic polarization P(**ω**)

$$[-\omega^2 + j\omega(\gamma + \frac{2}{T_2}) + \omega_a^2]\,\tilde{P}_x = \frac{Ne^2}{m}\tilde{E}_x$$

$$\boxed{\tilde{P}_x(\omega) = \frac{Ne^2}{m}\frac{\tilde{E}_x}{\omega_a^2 - \omega^2 + j\omega(\gamma + 2/T_2)}}$$

Susceptibility

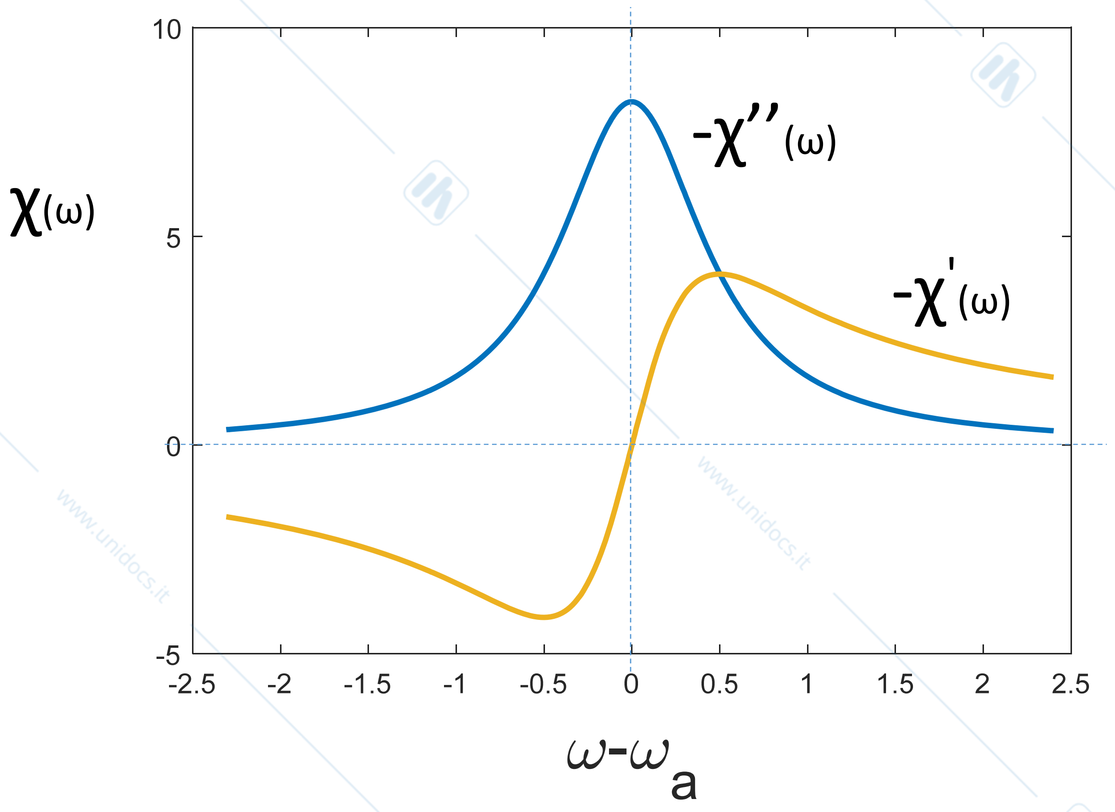
In a linear isotropic medium we can say that the Polarization is linearly proportional to the Electric field. Therefore we define the susceptibility χ(ω) as:

$$\mathbf{P}(\omega) = \chi(\omega)\varepsilon_0 E(\omega)$$

$$\chi(\omega) = \frac{Ne^2}{m\varepsilon}\frac{1}{\omega_a^2 - \omega^2 + j\omega\Delta\omega_a} = \chi'(\omega) + j\chi''(\omega)$$

$$\Delta\omega_a = \gamma + \frac{2}{T_2}$$

Susceptibility as function of ω



Important Note:

- In our analysis we have considered only N atoms in level E1 and zero atoms in level E2. Therefore we have χ''(ω)<0.

- In general, we N1 atoms at levels E1 and N2 atoms in level E2.
  Therefore we must substitute N=(N1-N2)
  - If N1>N2 => χ''(ω)<0
  - If N2>N1 => χ''(ω)>0

Physical meaning of χ’’(ω) and χ’(ω)

- A plane wave with electric field $E_0e^{j\omega t}$ propagating in the medium will “see” a “total” dialectic constant ε_{tot} given by:

$$\varepsilon_{tot} = \frac{D}{E} = \frac{\varepsilon E + P_{at}}{E} = \frac{\varepsilon E + \varepsilon_0 \chi E}{E} = \varepsilon(1 + \frac{\varepsilon_0}{\varepsilon}\chi)$$

Propagation constant in the medium

$$n = \sqrt{\frac{\varepsilon}{\varepsilon_0}} \qquad k = \omega\sqrt{\mu\varepsilon_{tot}}$$

Amplification (ie: gain) or absorption

$$k = \omega\sqrt{\mu\varepsilon}\sqrt{1 + \frac{1}{n^2}\chi} \approx \omega\sqrt{\mu\varepsilon_0}n(1 + \underbrace{\frac{1}{2n^2}}_{}\chi' + \boxed{\frac{i}{2n^2}\chi''}) = k_r + ik_i$$

Refractive index change

$$E = E_0e^{-i(k_r+ik_i)z} = E_0e^{-ik_rz}e^{k_iz} \Longrightarrow I(z) \propto e^{2k_iz}$$

The intensity of the electric field will increase in case N2>N1 or decrease in case N1>N2

Summary slide- We have learned that:

1) The interaction of the light with the semiconductor medium can be studied in the frame of the classical oscillator model
2) An applied electric field induces a macroscopic polarization obtained by averaging the microscopic dipoles
3) Microscopic dipole decay rate is dominated by radiative (and non-radiative) decay rate (γ), whereas the macroscopic polarization decay rate is also affected by the dephasing process. The polarization decay rate is dominated by the term 1/T2 at room temperature
4) The induced polarization is maximum (maximum of the imaginary part of the susceptibility) when the electric field pulsation is equal to the resonance pulsation ω_a
5) Next step is now examining how the electric field transfers (or absorbs) energy to (from) the atoms

How the electric field transfers the power to the atoms

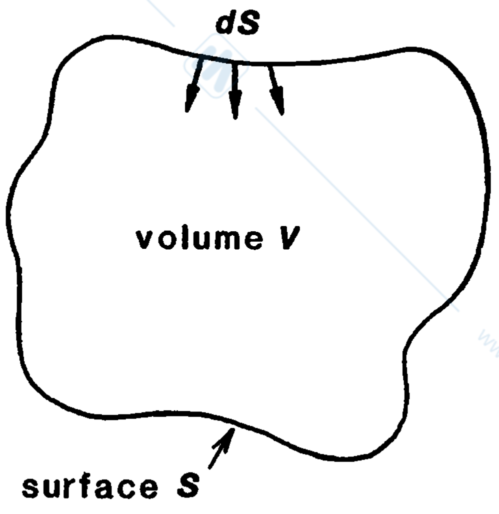


FIGURE 4.2
Volume V with a surface S for the evaluation of electromagnetic power flow.

Power flow

$$\overbrace{\int_S (\boldsymbol{\mathcal{E}} \times \boldsymbol{h}) \cdot d\boldsymbol{S}}^{1} = \overbrace{\frac{d}{dt} \int_V \left(\frac{1}{2} \epsilon_0 |\boldsymbol{\mathcal{E}}|^2 + \frac{1}{2} \mu_0 |\boldsymbol{h}|^2 \right) dV}^{2}$$

$$\underbrace{+ \int_V (\boldsymbol{\mathcal{E}} \cdot \boldsymbol{j})\, dV}_{3}$$

$$\underbrace{+ \int_V \left(\boxed{\boldsymbol{\mathcal{E}} \cdot \frac{d\boldsymbol{p}}{dt}} + \mu_0 \boldsymbol{h} \cdot \frac{d\boldsymbol{m}}{dt} \right) dV.}_{4}$$

We calculate this
term in next slide

Power flow

- (1) Integral of the (inwardly directed) Poynting vector => total electromagnetic power flowing into the volume V at any time instant
- (2) Instantaneous rate of the increase or decrease of the electromagnetic energy in the volume V
- (3) current contribution
- (4) instantaneous power per unit volume delivered by the fields to any dielectric ***(p)*** or magnetic ***(m)*** polarizations.

$$\mathcal{E}_x(t) = \tfrac{1}{2}\left[\tilde{E}_x e^{j\omega t} + \tilde{E}_x^* e^{-j\omega t}\right]$$

$$P_x(t) = \tfrac{1}{2}\left[\tilde{P}_x e^{j\omega t} + \tilde{P}_x^* e^{-j\omega t}\right]$$

$$\tilde{P}_x(\omega) = \chi(\omega)\varepsilon_0\tilde{E}_x = [\chi'(\omega) + j\chi''(\omega)]\varepsilon_0\tilde{E}_x$$

$$\left.\frac{dU_a}{dt}\right|_{averaged} = \frac{j\omega}{4}\left[\tilde{E}_x^*\tilde{P}_x - \tilde{E}_x\tilde{P}_x^*\right] = -\frac{1}{2}\varepsilon_0\omega\chi''^2(\omega)|\tilde{E}_x|^2$$

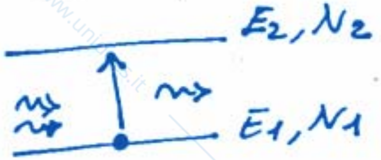
$\left.\frac{dU_a}{dt}\right|_{averaged} > 0$: atoms absorb energy from the field $\mathcal{E}_x(t)$ $\Rightarrow$
$\chi''(\omega) < 0 \Rightarrow$ ABSORPTION of LIGHT

$\left.\frac{dU_a}{dt}\right|_{averaged} < 0$: electric field absorb energy from the atoms
$\chi''(\omega) > 0 \Rightarrow$ STIMULATED EMISSION of LIGHT

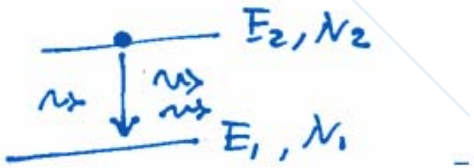
Stimulated emission and absorption

$U_a(t) = N_2 E_2 + N_1 E_1$ $\qquad N_2 + N_1 = N_{tot}$

$U_a(t) \nearrow \Rightarrow N_2 \nearrow$ and $N_1 \downarrow \Rightarrow$ ABSORPTION



$U_a(t) \swarrow \Rightarrow N_2 \downarrow$ and $N_1 \uparrow \Rightarrow$ STIMULATED EMISSION



Considering N2 atoms in state E2 and N1 atoms in state E1, let's calculate the total rate of variation of $U_a(t)$ (see next slide)

Net rate of variation of the total energy: dU_a/dt

$$\chi''(\omega) = -\frac{3}{4\pi^2}\frac{N\gamma_{rad}\lambda^3}{\Delta\omega_a}\frac{1}{1+\left[\frac{2(\omega-\omega_a)}{\Delta\omega_a}\right]^2}$$

$$\frac{dU_a}{dt} = \frac{3}{8\pi^2}\frac{N_1\gamma_{rad}\lambda^3}{\Delta\omega_a}\frac{\omega\varepsilon|\tilde{E}_x|^2}{1+\left[\frac{2(\omega-\omega_a)}{\Delta\omega_a}\right]^2} - \frac{3}{8\pi^2}\frac{N_2\gamma_{rad}\lambda^3}{\Delta\omega_a}\frac{\omega\varepsilon|\tilde{E}_x|^2}{1+\frac{4(\omega-\omega_a)^2}{\Delta^2\omega_a}}$$

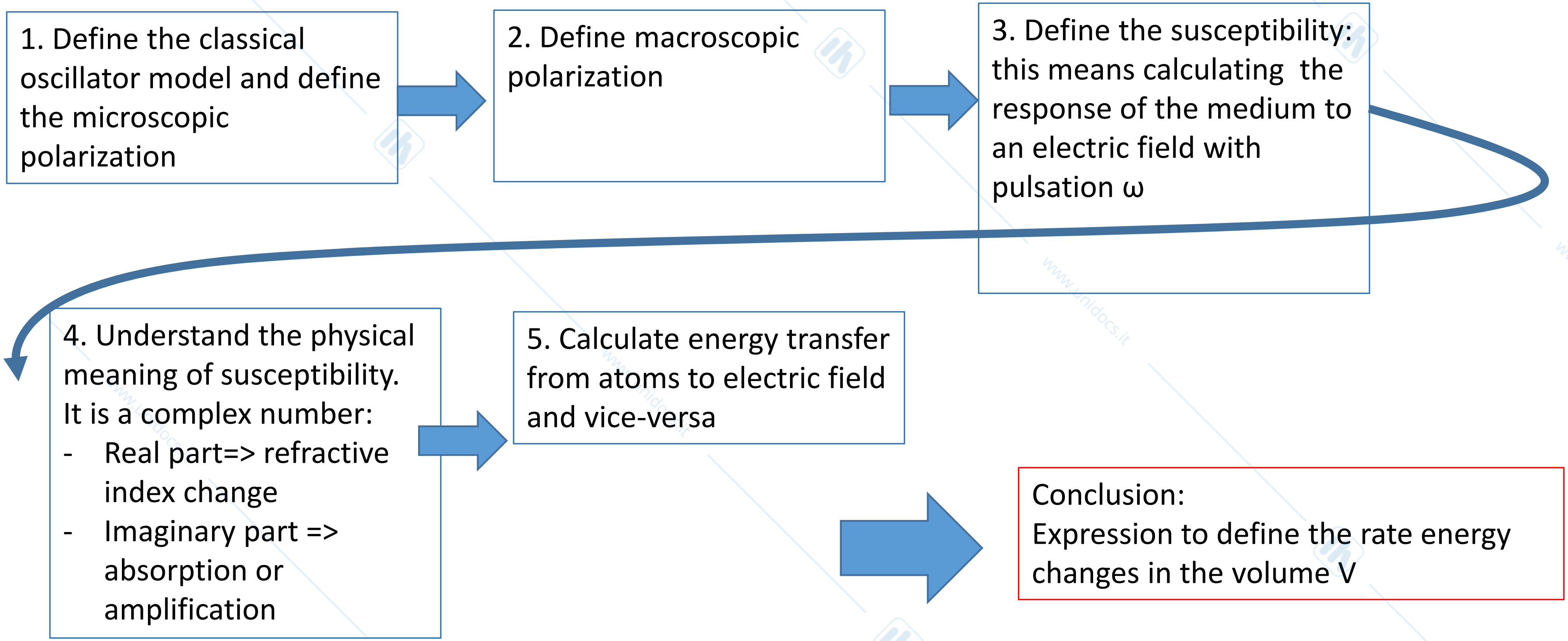
$$\frac{dU_a}{dt} = \left(\frac{3}{8\pi^2}\frac{\gamma_{rad}}{\Delta\omega_a}\frac{1}{\hbar}\hbar\omega_a|\tilde{E}_x|^2\right)(N_1-N_2) = W_{12}\hbar\omega_a N_1 - W_{21}\hbar\omega_a N_2$$

$$W_{12} = W_{21} = \frac{3}{8\pi^2}\frac{\gamma_{rad}}{\Delta\omega_a}\frac{1}{\hbar}|\tilde{E}_x|^2$$

Summary slide

- We have calculated the power transfer from the electric field to the atoms and vice-versa
- We have introduced the concept of absorption and stimulated emission rates

Map of main concepts of lesson B1



1. Define the classical oscillator model and define the microscopic polarization

2. Define macroscopic polarization

3. Define the susceptibility: this means calculating the response of the medium to an electric field with pulsation ω

4. Understand the physical meaning of susceptibility.
It is a complex number:
- Real part=> refractive index change
- Imaginary part => absorption or amplification

5. Calculate energy transfer from atoms to electric field and vice-versa

Conclusion:
Expression to define the rate energy changes in the volume V

LESSON B1- CONCLUSIONS

- We have studied the interaction of light with the semiconductor materials in the frame of the classical electron oscillator model (Lorentz's model)

- The light can transfer energy to the atoms (or valence band electrons) or receive energy from the atoms (or conduction band electrons). In the latter we have the stimulated emission of photons.

- Spontaneous emission, absorption and stimulated emission can be treated with a phenomenological model => the Rate Equation model.

Next LESSON B2

- Definition of gain and absorption coefficients
- Model for the calculation of the gain and absorption spectra
- Examples