University of Hamburg, Department of Physics Nonlinear Optics Kärtner/Mücke, WiSe 2017/2018 Problem Set 1

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1. Susceptibility tensor and symmetries.

Consider a two-dimensional medium with D_4 - symmetry (square). There is a set of symmetry operations, which leave the unit cell invariant:

- **E**: Identity operation
- \mathbf{R}_+ : Rotation by $\pi/2$
- \mathbf{R}_{-} : Rotation by $-\pi/2$

R: Rotation by π

 \mathbf{M}_x : Mirror image around the x-axis

- \mathbf{M}_y : Mirror image around the y-axis
- \mathbf{D}_1 : Mirror image around the diagonal \mathbf{D}_1

 \mathbf{D}_2 : Mirror image around the diagonals \mathbf{D}_2



Abbildung 1: D_4 -symmetry

A sequence of symmetry operations (e.g, two) is defined as the concatenation or product of the corresponding (two) operators. For example $M_x R_+ = D_2$. (a) Construct the multiplication table for the symmetry group:

	E	R_+	R_{-}	R	M_x	M_y	D_1	D_2
E								
R_+								
R_{-}								
R								
M_x								
M_y								
D_1								
D_2								

Tabelle 1: multiplication table for symmetry group ${\cal D}_4$

(b) The dielectric tensor of a general two-dimensional medium without symmetry has the form

$$\boldsymbol{\epsilon} = \left(\begin{array}{cc} \varepsilon_{11} & \varepsilon_{12} \\ \varepsilon_{21} & \varepsilon_{22} \end{array}\right)$$

Show that for a medium with D_4 -symmetry the dielectric tensor is isotropic

$$\boldsymbol{\epsilon} = \left(\begin{array}{cc} \varepsilon & 0 \\ 0 & \varepsilon \end{array} \right).$$

2. Coupled oscillator model



Abbildung 2: oscillator

Classical model for a nonlinear optical material, which has optical phonons that are at THz frequencies, i.e, the phonon or ions oscillation radiates an electro-magnetic wave in the THz range. The electron response dominates at high frequencies, while the ions' response dominates at low frequencies because of their higher mass. In order to consider the material response of the term $(x_i - x_e)^2$ from equation (1) and (2). Also, this $(x_i - x_e)^2$ interaction term can be understood as a potential of ions and electrons generate on each other.

We want to use this model to derive the susceptibilities for an artificial The phonon resonance frequency shall be at $f_i = 2$ THz, and its quality factor is $Q_i = 10$ (damping $\gamma_i = \frac{2\omega_i}{Q_i}$). In addition, the atoms in each unit cell of the material show electronic transitions at UV-frequencies $f_e = 1500$ THz with a a quality factor of $Q_e = 1000$ ($\gamma_e = \frac{2\omega_e}{Q_e}$). The material has a cubic unit cell with dimensions a=b=c=0.5 nm.

The emphasis of this problem is the THz frequency range by including the motion of the ion in the coupled oscillator model shown in equation (1) and (2) whereas the conventional Lorentz model neglects those resonances in the low frequency components and assumes them to be far apart from the optical frequencies meaning that it only considers the pure effect of the electrons response and is only valid when the external driving field is at high optical frequency.

The equations of motion for the electrons and phonons or ion positions in the material are

$$\ddot{x_i} + \omega_i^2 x_i + \gamma_i \dot{x_i} - \frac{\beta}{m_i} (x_i - x_e)^2 = \frac{I(E_1 e^{i(\omega_1 t - k_1 z)} + E_2 e^{i(\omega_2 t - k_2 z)})}{m_i}$$
(1)

$$\ddot{x_e} + \omega_e^2 x_e + \gamma_e \dot{x_e} + \frac{\beta}{m_e} (x_i - x_e)^2 = \frac{e(E_1 e^{i(\omega_1 t - k_1 z)} + E_2 e^{i(\omega_2 t - k_2 z)})}{m_e}$$
(2)

Equation (1) describes the motion of the ion, where I is the charge of the ion, and equation (2) describe the motion of the electron, where e is the charge of the electron; β is the coupling constant. All the needed constants are listed in table 2.

a) Derive a general frequency-dependent expression for the linear suszeptibility of the material at THz and optical frequencies due to the ionic and electronic contribution and discuss the result.

b) Give an expression for the frequency-independent linear susceptibility of the material at THz and optical frequencies when using it far below the corresponding resonance frequencies in the THz and optical domain, i.e. using Kleinman Symmetry.

c) Sketch the refractive index as a function of frequency on a logarithmic scale over the range from 0 to 1000 THz.

VOLUNTARY PART (d)

d) solve the $\chi^{(2)}$ for the difference frequency generation (e.g $\chi^{(2)}(\omega_1 - \omega_2, \omega_1, -\omega_2))$ and discuss it.

Quantity	ion	electron		
resonance frequency	$\omega_i = 2 * pi * 2 \text{THz}$	$\omega_e = 2 * pi * 1500 \text{THz}$		
quality factor	$Q_i = 10$	$Q_e = 1000$		
charge	$e = -1.6 * 10^{-19}C$	$I = 1.6 * 10^{-19}C$		
density $\approx a * b * c$	$N_i = 10^{28} m^{-3}$	$N_e = 10^{28} m^{-3}$		
coupling constant β	$10^9 kg * m^{-1} * s^{-2}$			

Tabelle 2: Variable table

Hint:

 $eN_ex_e = P_{linear} = \epsilon_0 \chi_e^{(1)} E$, where P_{linear} is the linear polarization term; $\omega_i \ll \omega_e;$

$$\chi^{(n)} = \chi_e^{(n)} + \chi_i^{(n)};$$

 ω_1, ω_2 is at the same order of magnitude as ω_0 ;

 $\omega_1 - \omega_2$ is at the same order of magnitude as ω_i .

Boyd chapter 1.4 discusses the Classical Anharmonic Oscillator. Although it is not coupled, you can take it is a starting point.