Final exam 2017-2018 for WMPH13004
Functional Properties - part on Optical materials
Friday 26 January 2018 (half of the 9:00-12:00 time slot)

This exam is drafted by the lecturer Caspar van der Wal, and reviewed by Graeme Blake

READ THIS FIRST:

- Clearly write your name and study number on each answer sheet that you use.
- On the first answer sheet, write the total number of answer sheets that you turn in.
- When turning in your answers, please stack your answer sheets in the proper order, and **staple** them together (stapler is at desk exam supervisors).
- Note that the last pages of these questions sheets list useful formulas and constants.
- The full exam is 90 points.

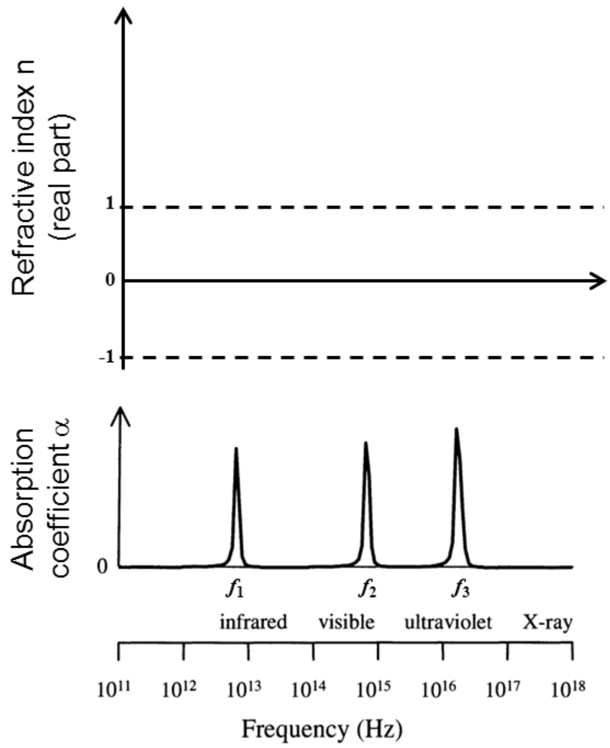
	Points per question and total									
Question	**1a**	**1b**	**1c**	**1d**	**2a**	**2b**	**3**	**4a**	**4b**	**4c**	**Total**
Points	8	6	8	8	8	10	18	8	8	8	**90**

The grade for this exam is calculated as: grade = 1 + 9 x (point score / 90).

Problem 1-opt

a) [8 points]

The lower panel of the following figure presents the absorption coefficient of a medium with electric dipole oscillators that behave as linear Lorentz oscillators. Copy the figure on your answer sheet, and sketch in the upper panel a graph of the refractive index *n* of this medium. There are no additional resonances at frequencies higher than f_3. Pay attention to details like how the trace in the graph should be with respect to the values of -1, 0 and 1, and the frequencies f_1, f_2, and f_3.



b) [6 points]
In the figure of question a), explain which of the features are (probably) due to electronic transitions and which ones are not. For the features that are not due to electronic transitions, explain what their origin can be instead.

c) [8 points]
For the figure of question a), explain what type of material this could be, by choosing one of these options:
- metal;
- semiconductor;
- crystalline insulator or glass;
- molecular material.

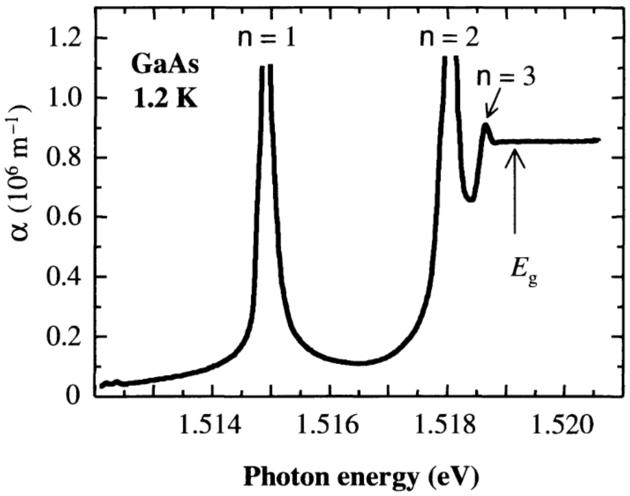
ALSO explain whether the material is doped / undoped / contains impurities.
For all parts of your answer, **explain your answer**.
NOTE: As long as you explain your answer, more than just one unique answer can be correct.

d) [8 points]
For the figure of question a), make an estimate for the index of refraction n for the frequency $f = 3 \times 10^{15}$ Hz. Use the information below here. ***First work your answer out in symbols, and fill in the numerical values as a last extra step of your answering.***
$f_1 = 8 \times 10^{12}$ Hz
$f_2 = 8 \times 10^{14}$ Hz
$f_3 = 2 \times 10^{16}$ Hz
Densities of oscillators (for the oscillators at frequencies f_1, f_2, f_3):
$N_1 = 3 \times 10^{27}$ m^{-3}
$N_2 = 4 \times 10^{28}$ m^{-3}
$N_3 = 5 \times 10^{29}$ m^{-3}

Problem 2-opt

a) [8 points]

The figure below here shows the absorption coefficient of a very pure piece of bulk GaAs at a temperature of 1.2 K. The peaks in the trace are due to the formation of free excitons. What is the value of the free-exciton binding energy? (This parameter is also known as the exciton Rydberg energy R_X.) The bulk bandgap value is marked as E_g. Explain your answer.



b) [10 points]

For the system that was introduced in question a), calculate the Bohr radius of the free exciton (that is, the exciton radius for $n = 1$).

Also calculate the effective mass for the holes that participate in the exciton formation.

Given parameters:

For the electron in GaAs the effective mass is $m_e^* = 0.067\ m_0$. For holes in GaAs the effective mass is $m_h^* = 0.2\ m_0$.

The relevant value of the dielectric constant (that is, the relative permittivity) is $\varepsilon_r = 12.8$.

The Rydberg energy for the hydrogen atom 13.6 eV, while the Bohr radius of this atom is 0.0529 nm

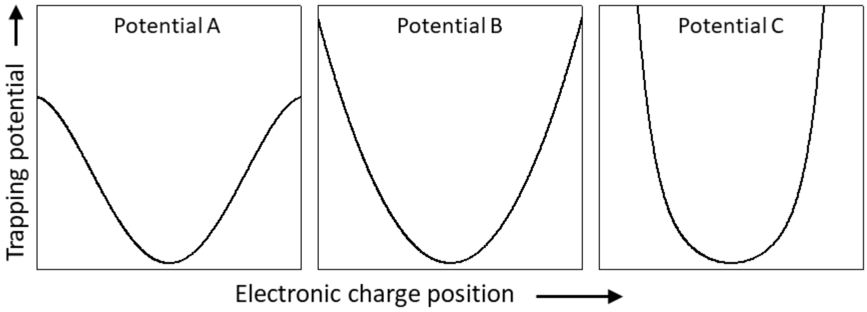
Problem 3-opt [18 points]

Explain, using energy diagrams, why the absorption band of a molecule is typically centered at a higher energy than the corresponding emission band.

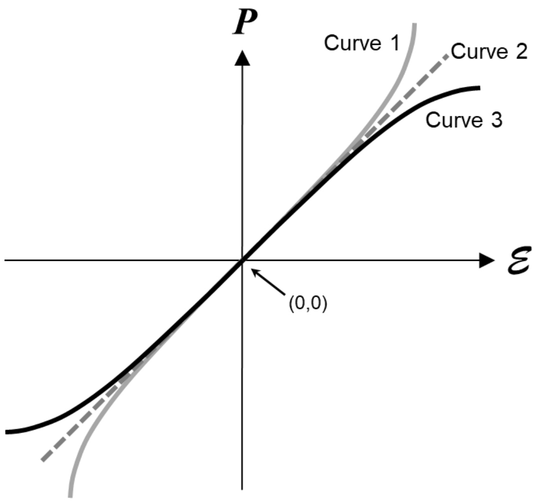
NOTE: Answer in at most half a page of text, if you want you can use extra space for adding a figure. A more complete answer gives more points.

Problem 4-opt

Consider three rather similar materials A, B and C, which all three only have electronic charges in localized states (trapped states, no free charge carriers). We will study the response to rather strong electromagnetic (EM) fields (which will possibly lead to nonlinear behavior), but the strength of the EM fields that we consider is never so strong that it leads to delocalization of charge carriers. The trapping potentials of the charge carriers that dominate the polarization response in the three materials are quite similar, but there are still some differences. The three trapping potentials (for electronic charge displacement along one relevant direction) for material A, B and C are plotted below here (all three plots are on the same scale).



For these three materials, the relation between the material's polarization ***P*** and the electric field $\mathcal{E}$ is represented by either *Curve 1*, *Curve 2* or *Curve 3* in the figure below here (all values of the curves are real numbers). The curves are valid for electric fields of UV light and all lower frequencies.



a) [8 points]
Which one of the three curves describes the properties of material A, which one that of B, and which one that of C? Explain your answer.

b) [8 points]
The electrical response of materials can be nonlinear for high $\mathcal{E}$. This can described by a nonlinear susceptibility $\chi^{\text{nonlinear}}$, which is usually described as a Taylor expansion around $\mathcal{E}$=0 where the first three terms have susceptibility coefficients $\chi^{(1)}$, $\chi^{(2)}$ and $\chi^{(3)}$. Consider *Curve 1*, *Curve 2* and *Curve 3* in the above figure. For each of the three curves, explain whether $\chi^{(1)}$, $\chi^{(2)}$ and $\chi^{(3)}$ are zero or non-zero, and what their sign is if non-zero.

c) [8 points]
Consider a material D (so, another material than A, B, C) that is described by *Curve 1* in the above figure. Show that when you apply a strong infrared laser beam of frequency ω to this material, that this will lead to the generation of EM fields at other frequencies than ω. *Also* clarify what the dominant frequencies are in the response of this material.

Useful formulas and constants

Fourier relations between t-representation and ω-representation of a phenomenon

$$x(t) \overset{\mathfrak{F}}{\leftrightarrow} X(\omega)$$

$$x(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} X(\omega)\, d\omega$$

$$X(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} x(t)\, dt$$

Trigonometric relations

$$\sin 2\theta = 2\sin\theta\cos\theta$$

$$\begin{aligned} \cos 2\theta &= \cos^2\theta - \sin^2\theta \\ &= 2\cos^2\theta - 1 \\ &= 1 - 2\sin^2\theta \end{aligned}$$

$$\sin 3\theta = 3\sin\theta - 4\sin^3\theta$$

$$\cos 3\theta = 4\cos^3\theta - 3\cos\theta$$

Optical coefficients

$$\tilde{n} = n + \mathrm{i}\kappa \qquad k = \tilde{n}\frac{\omega}{c} = (n + \mathrm{i}\kappa)\frac{\omega}{c}$$

$$\alpha = \frac{2\kappa\omega}{c} = \frac{4\pi\kappa}{\lambda}$$

$$\begin{aligned} \epsilon_1 &= n^2 - \kappa^2 \\ \epsilon_2 &= 2n\kappa\,, \end{aligned}$$

$$\begin{aligned} n &= \frac{1}{\sqrt{2}}\left(\epsilon_1 + (\epsilon_1^2 + \epsilon_2^2)^{1/2}\right)^{1/2} \\ \kappa &= \frac{1}{\sqrt{2}}\left(-\epsilon_1 + (\epsilon_1^2 + \epsilon_2^2)^{1/2}\right)^{1/2} \end{aligned}$$

Lorentz oscillators

$$\begin{aligned} \epsilon_1(\omega) &= 1 + \chi + \frac{Ne^2}{\epsilon_0 m_0}\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2} \\ \epsilon_2(\omega) &= \frac{Ne^2}{\epsilon_0 m_0}\frac{\gamma\omega}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}. \end{aligned}$$

Matrix element for optical transitions

$$M = \frac{e}{V}\int u_{\mathrm{f}}^*(\boldsymbol{r})\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}_{\mathrm{f}}\cdot\boldsymbol{r}}\,\left(\boldsymbol{\mathcal{E}}_0\cdot\boldsymbol{r}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\right)\,u_{\mathrm{i}}(\boldsymbol{r})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}_{\mathrm{i}}\cdot\boldsymbol{r}}\,\mathrm{d}^3\boldsymbol{r}$$

Excitons

$$E(n) = -\frac{\mu}{m_0}\frac{1}{\epsilon_{\mathrm{r}}^2}\frac{R_{\mathrm{H}}}{n^2} = -\frac{R_{\mathrm{X}}}{n^2} \qquad r_n = \frac{m_0}{\mu}\,\epsilon_{\mathrm{r}}\,n^2 a_{\mathrm{H}} = n^2 a_{\mathrm{X}}$$

Quantum confinement

$$E(n_x, n_y, n_z) = \frac{\pi^2 \hbar^2}{2m^*} \left(\frac{n_x^2}{d_x^2} + \frac{n_y^2}{d_y^2} + \frac{n_z^2}{d_z^2} \right)$$

Free electron plasma

$$\epsilon_r(\omega) = 1 - \frac{\omega_p^2}{(\omega^2 + i\gamma\omega)}$$

$$\omega_p = \left(\frac{Ne^2}{\epsilon_0 m_0} \right)^{1/2} .$$

Frequently used constants

Quantity	Symbol	Value	Unit	Relative std. uncert. u_r
speed of light in vacuum	c, c_0	299 792 458	$\mathrm{m\,s^{-1}}$	(exact)
magnetic constant	μ_0	$4\pi \times 10^{-7}$	$\mathrm{N\,A^{-2}}$	
		$= 12.566\,370\,614... \times 10^{-7}$	$\mathrm{N\,A^{-2}}$	(exact)
electric constant $1/\mu_0 c^2$	ϵ_0	$8.854\,187\,817... \times 10^{-12}$	$\mathrm{F\,m^{-1}}$	(exact)
Newtonian constant of gravitation	G	$6.674\,28(67) \times 10^{-11}$	$\mathrm{m^3\,kg^{-1}\,s^{-2}}$	1.0×10^{-4}
Planck constant	h	$6.626\,068\,96(33) \times 10^{-34}$	J s	5.0×10^{-8}
$h/2\pi$	$\hbar$	$1.054\,571\,628(53) \times 10^{-34}$	J s	5.0×10^{-8}
elementary charge	e	$1.602\,176\,487(40) \times 10^{-19}$	C	2.5×10^{-8}
magnetic flux quantum $h/2e$	Φ_0	$2.067\,833\,667(52) \times 10^{-15}$	Wb	2.5×10^{-8}
conductance quantum $2e^2/h$	G_0	$7.748\,091\,7004(53) \times 10^{-5}$	S	6.8×10^{-10}
electron mass	m_e	$9.109\,382\,15(45) \times 10^{-31}$	kg	5.0×10^{-8}
proton mass	m_p	$1.672\,621\,637(83) \times 10^{-27}$	kg	5.0×10^{-8}
proton-electron mass ratio	m_p/m_e	$1836.152\,672\,47(80)$		4.3×10^{-10}
fine-structure constant $e^2/4\pi\epsilon_0\hbar c$	α	$7.297\,352\,5376(50) \times 10^{-3}$		6.8×10^{-10}
inverse fine-structure constant	α^{-1}	$137.035\,999\,679(94)$		6.8×10^{-10}
Rydberg constant $\alpha^2 m_e c/2h$	R_∞	$10\,973\,731.568\,527(73)$	$\mathrm{m^{-1}}$	6.6×10^{-12}
Avogadro constant	N_A, L	$6.022\,141\,79(30) \times 10^{23}$	$\mathrm{mol^{-1}}$	5.0×10^{-8}
Faraday constant $N_A e$	F	$96\,485.3399(24)$	$\mathrm{C\,mol^{-1}}$	2.5×10^{-8}
molar gas constant	R	$8.314\,472(15)$	$\mathrm{J\,mol^{-1}\,K^{-1}}$	1.7×10^{-6}
Boltzmann constant R/N_A	k	$1.380\,6504(24) \times 10^{-23}$	$\mathrm{J\,K^{-1}}$	1.7×10^{-6}
Stefan-Boltzmann constant $(\pi^2/60)k^4/\hbar^3 c^2$	σ	$5.670\,400(40) \times 10^{-8}$	$\mathrm{W\,m^{-2}\,K^{-4}}$	7.0×10^{-6}
	Non-SI units accepted for use with the SI			
electron volt: (e/C) J	eV	$1.602\,176\,487(40) \times 10^{-19}$	J	2.5×10^{-8}
(unified) atomic mass unit $1\,\mathrm{u} = m_u = \frac{1}{12}m(^{12}\mathrm{C}) = 10^{-3}\,\mathrm{kg\,mol^{-1}}/N_A$	u	$1.660\,538\,782(83) \times 10^{-27}$	kg	5.0×10^{-8}