

Wavepropagation in layered structures  
Optical filters

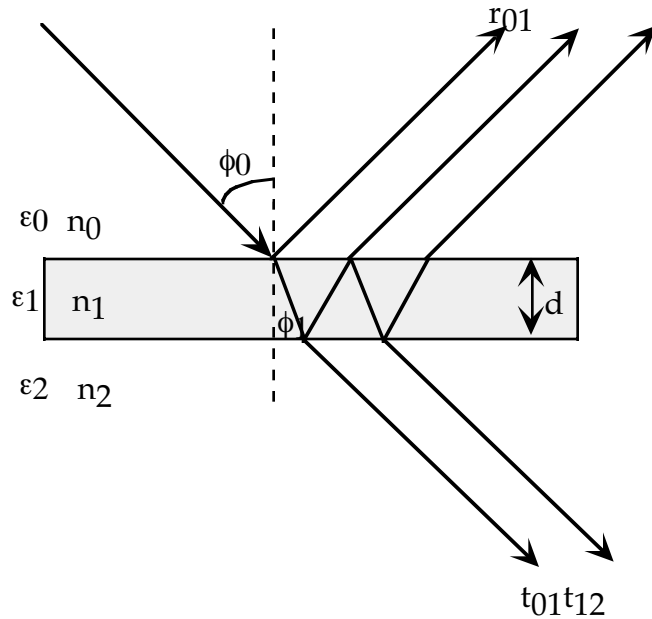
by

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## REFLECTION AND TRANSMISSION

The starting point for our discussion is Maxwell's equations. These lead to the boundary conditions saying that the tangential components of  $\vec{E}$  og  $\vec{H}$  are continuous across a boundary. These conditions lead for example to Fresnel's formulas for the reflection from a single boundary.

We will now look at the reflection from a thin film on a substrate. The system is illustrated in the figure below.



The incident wave  $E_i$  hits the first interface. Some is reflected from the first interface, some is transmitted and then reflected at the second interface etc. We get a sum of partial waves (NB we are summing field amplitudes)

$$r = r_{01} + t_{01}r_{12}t_{10}e^{2i\delta_1} + t_{01}r_{12}r_{10}r_{12}t_{10}e^{4i\delta_1} + \dots$$

$$= r_{01} + \frac{r_{12}t_{01}t_{10}e^{2i\delta_1}}{1 + r_{12}r_{01}e^{2i\delta_1}}$$

$$t = t_{01}t_{12}e^{i\delta_1} + t_{01}r_{12}r_{10}t_{12}e^{3i\delta_1} + \dots$$

$$= \frac{t_{01}t_{12}e^{i\delta_1}}{1 + r_{12}r_{01}e^{2i\delta_1}}$$

We use Fresnel's equations to simplify the expression for  $r$

$$r = \frac{r_{01} + (r_{01}^2 r_{12} + r_{12} t_{01} t_{10} e^{2i\delta_1})}{1 + r_{12} r_{01} e^{2i\delta_1}}$$

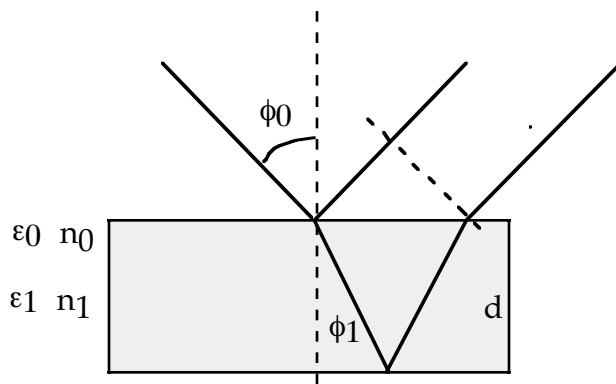
From Fresnel's formulas you can show that  $r_{01}^2 + t_{01} t_{10} = 1$ . This leads to

$$r = \frac{r_{01} + r_{12} e^{2i\delta_1}}{1 + r_{12} r_{01} e^{2i\delta_1}} \quad \text{Show this yourself!}$$

$2\delta_1$  is the phase difference between waves 1 and 2. From the optical path difference we get

$$\delta_1 = \frac{2\pi}{\lambda} n_1 d_1 \cos \varphi_1$$

Proof:



The difference in optical path length ( $n$  times geometrical path length):

$$\begin{aligned} & \frac{n_1 2d}{\cos \phi_1} - 2d \operatorname{tg} \phi_1 \sin \phi_0 n_0 \\ &= 2d \left( \frac{n_1}{\cos \phi_1} - \operatorname{tg} \phi_1 \sin \phi_0 n_0 \right) \\ &= 2d \left( \frac{n_1}{\cos \phi_1} - \frac{\sin \phi_1}{\cos \phi_1} n_1 \sin \phi_1 \right) = 2dn_1 \cos \phi_1 \end{aligned}$$

This gives  $\delta_1 = \frac{2\pi}{\lambda} n_1 d_1 \cos \varphi_1$ .

$r_{01}$  and  $r_{12}$  are the reflection coefficients at the 0,1 and 1,2 interfaces. They are given by Fresnel's formulae.



A double film can now be solved by recursion. We then replace the reflection from the back side by the reflection from a film-covered surface

$$r = \frac{r_{01} + \rho e^{2i\delta_1}}{1 + \rho \cdot r_{01} e^{2i\delta_1}}$$

Where  $\rho = \frac{r_{12} + r_{23} e^{2i\delta_2}}{1 + r_{12} \cdot r_{23} e^{2i\delta_2}}$

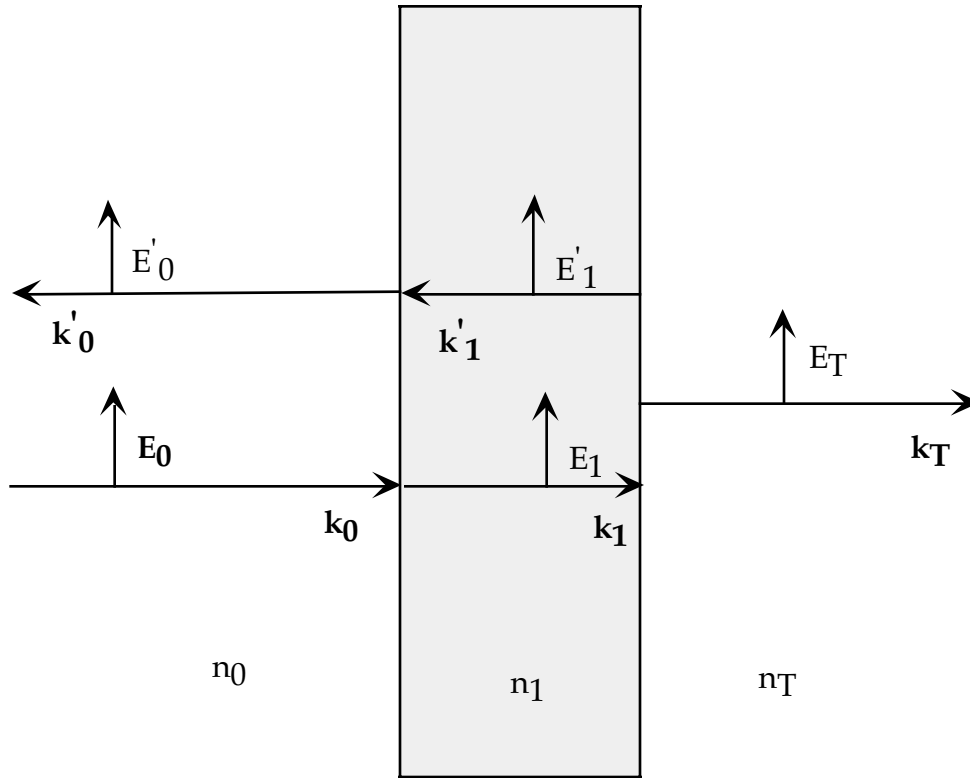
Is inserted:

$$r = \frac{r_{01} + r_{12} e^{2i\delta_1} + r_{23} e^{2i(\delta_1 + \delta_2)} + r_{01} r_{12} r_{23} e^{2i\delta_2}}{1 + r_{01} r_{12} e^{2i\delta_1} + r_{01} r_{23} e^{2i(\delta_1 + \delta_2)} + r_{12} \cdot r_{23} e^{2i\delta_2}}$$

This is becoming somewhat complicated for many layers. We will turn to transfer matrix theory. This is a better solution for a system containing many layers.

## MATRIX THEORY FOR FILMS

We will first develop an expression for the transfer matrix for a single film on a substrate. Look at the following situation:



We have a film of thickness  $d$ . The system consists of a wave with an incident field vector  $\bar{E}_0$  and incident  $\bar{k}$ -vector equal  $\bar{k}_0$ , a reflected wave in the first medium, a transmitted and reflected field in the second medium a transmitted wave in the third medium. We use the continuity equations at the interfaces

$E_{\text{tang}}$  is continuous,  $H_{\text{tang}}$  is continuous. Furthermore from Maxwell's equations:

$$\bar{k} \times \bar{E} = \mu\omega \bar{H} \Rightarrow H = Z_0^{-1} n \cdot E \quad Z_0 \text{ is the so-called surface impedance}$$

$n$  is the refractive index.

The continuity equations used on the first interface give:

$$E_0 + E_0' = E_1 + E_1' \quad (\text{I})$$

$$H_0 - H_0' = H_1 - H_1' \quad (\text{NB! The direction of } \bar{H} \text{ is give by the direction of } \bar{E})$$

We use  $H \propto nE \Rightarrow$

$$n_0 E_0 - n_0 E_0' = n_1 E_1 - n_1 E_1' \quad (\text{II})$$

Second interface:

$$E_1 e^{ik_1 d} + E_1' e^{-ik_1 d} = E_T \quad (\text{III})$$

$$H_1 e^{ik_1 d} - H_1' e^{-ik_1 d} = H_T$$

$$n_1 E_1 e^{ik_1 d} - n_1 E_1' e^{-ik_1 d} = n_T E_T \quad (\text{IV})$$

We solve the equations (I) - (IV) for  $E_0'$  and  $E_T$ , after rearranging as follows

$$\text{III: } (E_1 + E_1') \cos k_1 d + (E_1 - E_1') i \sin k_1 d = E_T$$

$$\text{IV: } n_1 (E_1 - E_1') \cos k_1 d + n_1 (E_1 + E_1') i \sin k_1 d = n_T E_T$$

We eliminate the fields inside the film by first solving for  $E_0' + E_0$  and  $E_0 - E_0'$ .

This gives:

$$1 + \frac{E_0'}{E_0} = (\cos k_1 d - i \frac{n_T}{n_1} \sin k_1 d) \frac{E_T}{E_0}$$

$$n_0 - n_0 \frac{E_0'}{E_0} = (-i n_1 \sin k_1 d + n_T \cos k_1 d) \frac{E_T}{E_0}$$

Written in matrix form

$$\begin{bmatrix} 1 \\ n_0 \end{bmatrix} + \begin{bmatrix} 1 \\ -n_0 \end{bmatrix} \frac{E_0'}{E_0} = \begin{bmatrix} \cos k_1 d & \frac{-i}{n_1} \sin k_1 d \\ -i n_1 \sin k_1 d & \cos k_1 d \end{bmatrix} \begin{bmatrix} 1 \\ n_T \end{bmatrix} \frac{E_T}{E_0}$$

But  $\frac{E_0'}{E_0}$  is just the reflection coefficient  $r$  and  $E_T/E_0$  is the transmission coefficient  $t$

$$\begin{bmatrix} 1 \\ n_0 \end{bmatrix} + \begin{bmatrix} 1 \\ -n_0 \end{bmatrix} r = \overline{\overline{M}} \begin{bmatrix} 1 \\ n_T \end{bmatrix} t$$

$$\overline{\overline{M}} = \begin{bmatrix} \cos k_1 d & \frac{-i}{n_1} \sin k_1 d \\ -i n_1 \sin k_1 d & \cos k_1 d \end{bmatrix}$$

is the transfer matrix for one film. For a system of many films the total transfer matrix is just a product of matrices

$$\begin{bmatrix} 1 \\ n_0 \end{bmatrix} + \begin{bmatrix} 1 \\ -n_0 \end{bmatrix} r = \overline{\overline{M}}_1 \overline{\overline{M}}_2 \overline{\overline{M}}_3 \overline{\overline{M}}_4 \dots \overline{\overline{M}}_n \begin{bmatrix} 1 \\ n_T \end{bmatrix} t$$

We can thus easily calculate r and t for complex systems by multiplying 2x2 matrices.

Each matrix is of the form

$$\overline{\overline{M}}_i = \begin{bmatrix} \cos k_i d_i & \frac{-i}{n_i} \sin k_i d_i \\ -i n_i \sin k_i d_i & \cos k_i d_i \end{bmatrix}$$

and the product of the form  $\overline{\overline{M}} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$

This gives

$$\begin{bmatrix} 1 \\ n_0 \end{bmatrix} + \begin{bmatrix} 1 \\ -n_0 \end{bmatrix} r = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} 1 \\ n_T \end{bmatrix} t$$

or after performing the matrix -vector multiplication

$$1 + r = (A + n_T B)t$$

$$n_0(1 - r) = (C + n_T D)t$$

Solved for r and t we get:

$$r = \frac{An_0 + Bn_0 n_T - C - Dn_T}{An_0 + Bn_0 n_T + C + Dn_T}$$

$$t = \frac{2n_0}{An_0 + Bn_0 n_T + C + Dn_T}$$

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The physics behind the matrix formalism is easier to see if we write it on the following form:

$$\begin{bmatrix} E_0 \\ H_0 \end{bmatrix} + \begin{bmatrix} E_0' \\ H_0' \end{bmatrix} = \overline{\overline{M}} \begin{bmatrix} E_T \\ H_T \end{bmatrix}$$

$E_0 + E_0' = E_0^I$  is the total field at surface I.....

$$\begin{bmatrix} E_0^I \\ H_0^I \end{bmatrix} = \overline{\overline{M}} \begin{bmatrix} E_T \\ H_T \end{bmatrix}$$

The transfer matrix thus transfers the total field from one interface to the next.

For non-normal incidence we can develop the equivalent theory. We start with a wave incident at an angle  $\varphi$ . The boundary conditions are the same, *the tangential component of E and H are continuous*.

Here we must distinguish between two cases, s- and p- polarised waves. S-polarised has its E-vector normal to the plane of incidence, p-polarised has its E-vector in the plane of incidence. The result is:

p-polarisation:

$$\begin{bmatrix} \cos \varphi_0 \\ n_0 \end{bmatrix} + \begin{bmatrix} \cos \varphi_0 \\ -n_0 \end{bmatrix} r = \overline{\overline{M}}_p \begin{bmatrix} \cos \varphi_T \\ n_T \end{bmatrix} t$$

with

$$\overline{\overline{M}}_p = \begin{bmatrix} \cos \beta & \frac{-i}{p} \sin \beta \\ -ip \sin \beta & \cos \beta \end{bmatrix}$$

$$\beta = k_1 d \cos \varphi_1 \quad p = n_1 / \cos \varphi_1$$

$n_1$  is the refractive index of the film

$\varphi_1$  is the propagation direction in the film

This finally gives:

$$r_p = \frac{A n_0 \cos \varphi_T + B n_0 n_T - C \cos \varphi_0 \cos \varphi_T - D n_T \cos \varphi_0}{A n_0 \cos \varphi_T + B n_0 n_T + C \cos \varphi_0 \cos \varphi_T + D n_T \cos \varphi_0}$$

and a corresponding equation for  $t_p$ .

For s polarisation:

$$\begin{bmatrix} 1 \\ n_0 \cos \varphi_0 \end{bmatrix} + \begin{bmatrix} 1 \\ -n_0 \cos \varphi_0 \end{bmatrix} r = \overline{\overline{M}}_s \begin{bmatrix} 1 \\ n_T \cos \varphi_T \end{bmatrix} t$$

$\overline{\overline{M}}_s$  has the same form as  $\overline{\overline{M}}_p$ , but with

$$\beta = k_1 d \cos \varphi_1 \quad p = n_1 \cos \varphi_1$$

and



$$r_s = \frac{An_0 \cos \varphi_0 + Bn_0 n_T \cos \varphi_0 \cos \varphi_T - C - Dn_T \cos \varphi_T}{An_0 \cos \varphi_0 + Bn_0 n_T \cos \varphi_0 \cos \varphi_T + C + Dn_T \cos \varphi_T}$$

In the limit  $d \Rightarrow 0$  blir  $A = D = 1, B = C = 0$

$$r_p = \frac{n_0 \cos \varphi_T - n_T \cos \varphi_0}{n_0 \cos \varphi_T + n_T \cos \varphi_0}$$

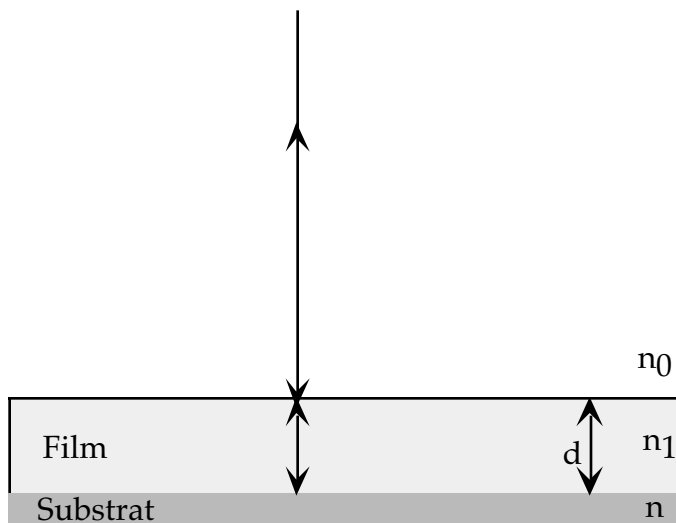
$$r_s = \frac{n_0 \cos \varphi_0 - n_T \cos \varphi_T}{n_0 \cos \varphi_0 + n_T \cos \varphi_T}$$

This is nothing but Fresnels formulas for a film-free surface

### ANTIREFLECTION COATING

WE will now use this theory on some relevant systems

A simple antireflection coating is shown in the figure. We assume normal incidence. The we know that:



$$r = \frac{An_0 + Bnn_0 - C - Dn}{An_0 + Bnn_0 + C + Dn}$$

$$A = \cos k_1 d$$

$$C = -in_1 \sin k_1 d$$

$$B = \frac{-i}{n_1} \sin k_1 d$$

$$D = A$$

Inserted:

$$r = \frac{n_1(n_0 - n) \cos kd - i(nn_0 - n_1^2) \sin kd}{n_1(n_0 + n) \cos kd - i(nn_0 + n_1^2) \sin kd}$$

We take  $d = \lambda/4 \rightarrow \cos kd = 0, \sin kd = 1.0$

This gives:

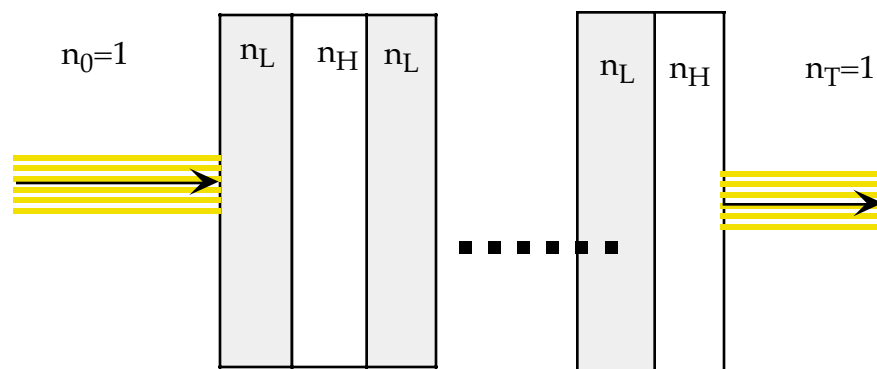
$$r = \frac{(nn_0 - n_1^2)}{(nn_0 + n_1^2)}$$

When  $n_1 = \sqrt{n_0 n}$ ,  $r = 0$

This is the fundamentals of anti-reflection coatings. This simple system is only good for  $\perp$  incidence and due to dispersion only for one  $\lambda$ . To get a wide band anti-reflection coating we must use a multilayer coating.

### HIGH-REFLECTANCE COATINGS

For lasers we need coatings with high reflectance. Look at the following system



We take system with high/low/high/low.....refractive index. For such a system we have:

$$\bar{\bar{M}}_i = \begin{bmatrix} \cos k_i d_i & \frac{-i}{n_i} \sin k_i d_i \\ -i n_i \sin k_i d_i & \cos k_i d_i \end{bmatrix}$$

Let us choose a system where each layer has an optical thickness of a quarter wavelength:  $k_i d_i = \pi/2$ .

$$\bar{\bar{M}}_i = \begin{bmatrix} 0 & \frac{-i}{n_i} \\ -i n_i & 0 \end{bmatrix}$$

For  $2N$  layers we get a total transfer matrix:

$$\bar{\bar{M}} = \begin{bmatrix} 0 & \frac{-i}{n_L} \\ -i n_L & 0 \end{bmatrix} \begin{bmatrix} 0 & \frac{-i}{n_H} \\ -i n_H & 0 \end{bmatrix} \begin{bmatrix} 0 & \frac{-i}{n_L} \\ -i n_L & 0 \end{bmatrix} \begin{bmatrix} 0 & \frac{-i}{n_H} \\ -i n_H & 0 \end{bmatrix} \cdots \begin{bmatrix} 0 & \frac{-i}{n_H} \\ -i n_H & 0 \end{bmatrix}$$

The product of two neighbouring matrices is of the form

$$\bar{\bar{P}} = \begin{bmatrix} -n_H / n_L & 0 \\ 0 & -n_L / n_H \end{bmatrix}$$

This is diagonal and the product of  $2N$  matrices then becomes

$$\bar{\bar{M}}_{2N} = \begin{bmatrix} -n_H / n_L & 0 \\ 0 & -n_L / n_H \end{bmatrix}^N = \begin{bmatrix} (-n_H / n_L)^N & 0 \\ 0 & (-n_L / n_H)^N \end{bmatrix}$$

For the reflection coefficient this becomes:

$$r = \frac{(-n_H / n_L)^N - (-n_L / n_H)^N}{(-n_H / n_L)^N + (-n_L / n_H)^N}$$

and the intensity reflection coefficient  $R$

$$R = r^2 = \left[ \frac{1 - (n_L / n_H)^{2N}}{1 + (n_L / n_H)^{2N}} \right]^2$$

We see directly that  $R \rightarrow 1$  when  $N$  is large.

WE have not included the substrate in this calculation. If we do, we will find that the reflectivity depends upon which film is the first; the high index or the low index film. If we start with a low index film and include the substrate the final result is:

$$R = r^2 = \left[ \frac{A - Dn_T}{A + Dn_T} \right]^2 = \left[ \frac{1 - (n_L/n_H)^{2N} n_T}{1 + (n_L/n_H)^{2N} n_T} \right]^2$$

Starting with a high index film we get:

$$R = r^2 = \left[ \frac{A - Dn_T}{A + Dn_T} \right]^2 = \left[ \frac{1 - (n_H/n_L)^{2N} n_T}{1 + (n_H/n_L)^{2N} n_T} \right]^2$$

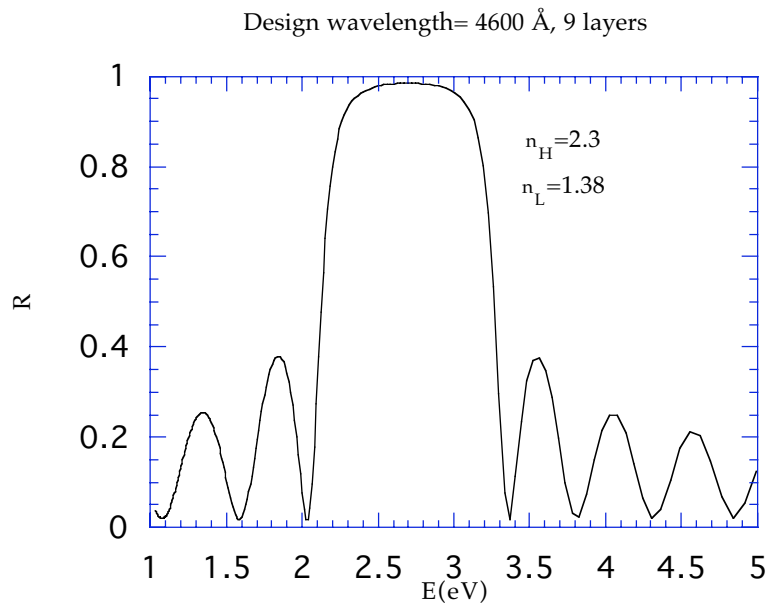
From this we see that it pays to start with the high index film

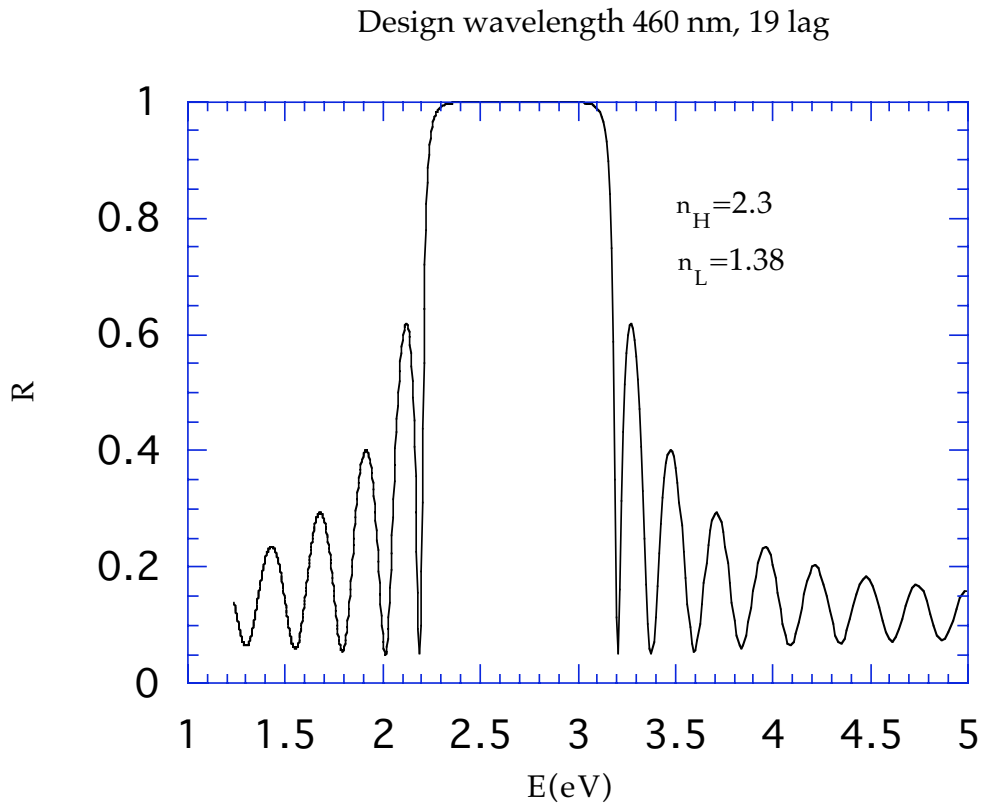
The bandwidth of the filter can be shown to be given by the expression

$$\sin \frac{\pi}{2} \frac{\Delta\lambda}{\lambda} = \pm \frac{n_a - n_b}{n_b + n_a} \cong \sin \frac{\pi}{2} \frac{\Delta\lambda}{\lambda_0} \quad \text{da } \lambda \approx \lambda_0$$

where  $\Delta\lambda$  is the bandwidth.

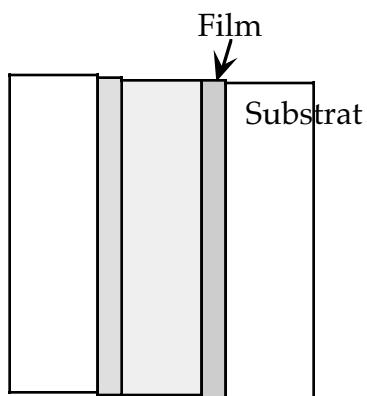
The figures below show two high reflectance filters with 9 and 19 layers respectively.





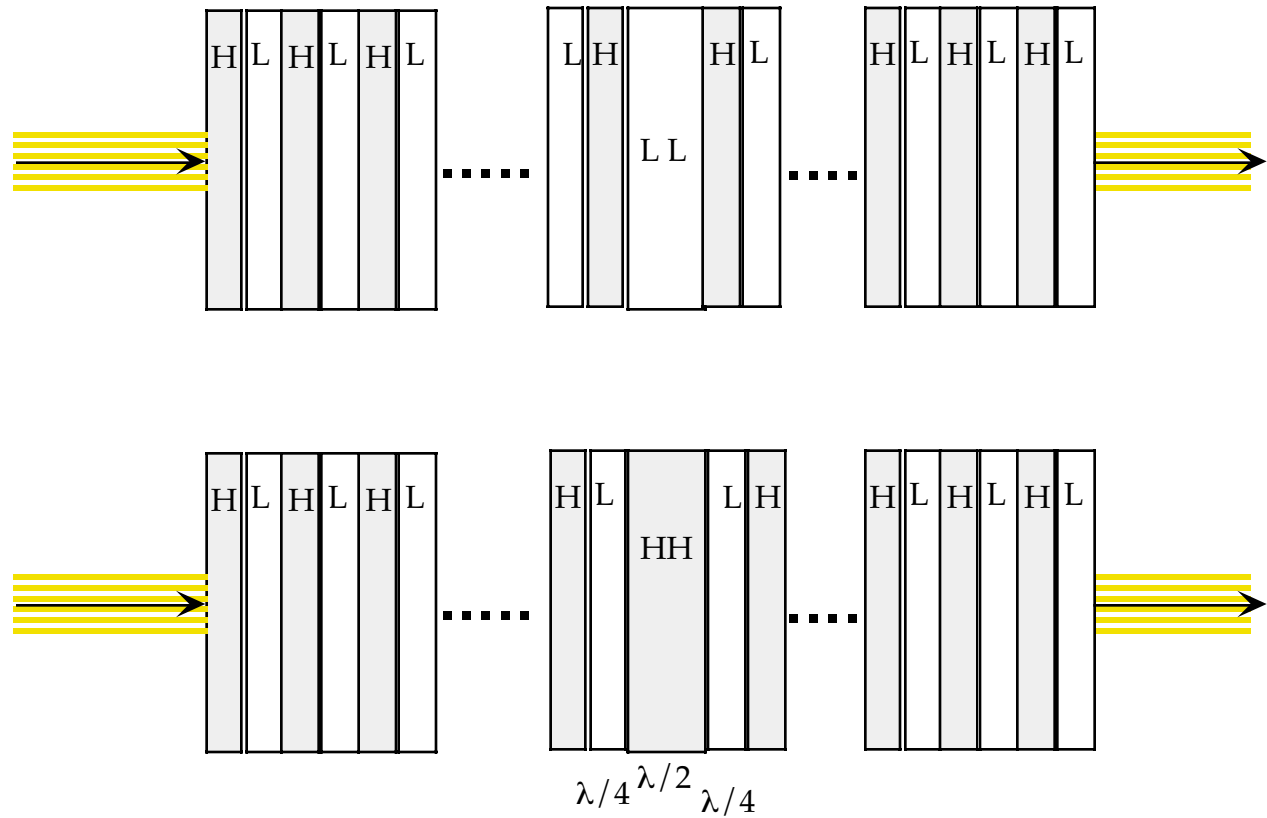
## BANDPASS FILTERS

A typical bandpass filter consist of two high reflectance filters and a Fabry Perot interferometer; see the figure.



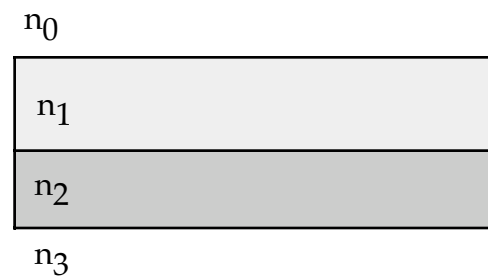
## POSSIBLE BANDPASS STRUCTURES

Possible configurations are given in the figure



## MORE ANTIREFLECTION COATINGS

An example is given in the figure.



$$M = \begin{bmatrix} -n_2/n_1 & 0 \\ 0 & -n_1/n_2 \end{bmatrix}$$

$$r = \frac{n_o \frac{n_2}{n_1} - n_3 \frac{n_1}{n_2}}{n_o \frac{n_2}{n_1} + n_3 \frac{n_1}{n_2}}$$

$$r = 0 \Rightarrow \frac{n_2^2}{n_1^2} = \frac{n_3}{n_o}$$

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The advantage is a higher bandwidth compared to a single film. Another possible structure is:

$$\frac{\lambda}{4} \quad \frac{\lambda}{2} \quad \frac{\lambda}{4} \quad \text{substrat.}$$

Eks.: MgF<sub>2</sub> ZrO<sub>2</sub> CeF<sub>3</sub> on glas

$$n = 1.37 \quad 2.1 \quad 1.63$$

## THE INTERACTION BETWEEN ELECTROMAGNETIC RADIATION AND MATTER

We will now discuss the interaction between radiation and matter. The general properties of the response function comes from the fact that the response is causal; i.e. the response depends only on the past and not on the future. This general statement leads to the so-called Kramers Kronig relations.

From causality we can write

$$\bar{D}(t) = \epsilon_0 \bar{E}(t) + \bar{P}(t)$$

$\bar{P}(t)$  is the total response of the system and it depends only on the past. Thus:

$$\bar{P}(t) = \epsilon_0 \int_0^{\infty} f(\tau) \bar{E}(t-\tau) d\tau = \epsilon_0 \int_{-\infty}^{\infty} f(\tau) \bar{E}(t-\tau) d\tau \quad \text{med } f(\tau)=0 \text{ for } \tau < 0$$

$f(\tau)$  is the response. It is zero for times in the future and this is reflected in the way we wrote the integral.  $t = 0$  is now,  $t = \infty$  is  $\infty$  past.  $f(\infty) = 0$ .

If we Fourier-transform the equation we get:

$$\bar{D}(t) = \int_{-\infty}^{\infty} d\omega \bar{D}(\omega) e^{-i\omega t}$$

$$\bar{E}(t-\tau) = \int_{-\infty}^{\infty} d\omega \bar{E}(\omega) e^{-i\omega t} \cdot e^{i\omega\tau}$$

Inserted in the first equation, we get

$$\bar{D}(\omega) = \epsilon_0 \bar{E}(\omega) + \epsilon_0 \bar{E}(\omega) \int_{-\infty}^{\infty} f(\tau) e^{i\omega\tau} d\tau$$

$$\epsilon_r(\omega) = 1 + \int_{-\infty}^{\infty} f(\tau) e^{i\omega\tau} d\tau$$

$\epsilon$  is the dielectric constant. It can be complex  $\epsilon_r(\omega) = \epsilon_1 + i\epsilon_2$ .

From the equation we see that

$$\epsilon_r^* = 1 + \int_{-\infty}^{\infty} f(\tau) e^{-i\omega\tau} d\tau$$

This means that

$$\epsilon_1(\omega) - i\epsilon_2(\omega) = \epsilon_1(-\omega) + i\epsilon_2(-\omega)$$

From causality we see that the real part is symmetric in  $\omega$ , the imaginary part is anti-symmetric.  $\epsilon-1$  is an analytic function in the complex upper half  $\omega$  plane..  $\epsilon-1 \rightarrow 0$  when  $\omega \rightarrow i\infty$  since only  $\tau > 0$  contributes.

We will now calculate the Cauchy integral

$$\int_{-\infty}^{\infty} \frac{\epsilon(\omega) - 1}{\omega - \omega_1} d\omega = I$$

$I = 0$  because  $\epsilon(\omega) - 1$  is regular in the upper half plane.

This can be written as: Residue in  $\omega = \omega_1 + P \int_{-\infty}^{\infty} = 0$ , and the residue contribution becomes  $-i\pi(\epsilon(\omega_1) - 1)$ . Rearranging we obtain the expression



$$\varepsilon(\omega_1) - 1 = \frac{1}{i\pi} \text{P} \int_{-\infty}^{\infty} \frac{\varepsilon(\omega) - 1}{\omega - \omega_1} d\omega$$

We change integration variables, write out explicitly the real and imaginary parts and get the Kramers Kronig relations in the form:

$$\varepsilon_1(\omega) = 1 + \frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\varepsilon_2(\xi)}{\xi - \omega} d\xi$$

$$\varepsilon_2(\omega) = \frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\varepsilon_1(\xi)}{\xi - \omega} d\xi$$

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P stands for "principal value" and we often write  $2 \times \int_0^{\infty}$  instead of as above. Doing that we get the Kramers Kronig relations in the form:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} \text{P} \int_0^{\infty} \frac{\xi \varepsilon_2(\xi)}{\xi^2 - \omega^2} d\xi$$

$$\varepsilon_2(\omega) = \frac{2}{\pi} \text{P} \int_0^{\infty} \frac{\omega \varepsilon_1(\xi)}{\xi^2 - \omega^2} d\xi$$

Causality means that if we can measure say the real part of a function for all frequencies, then we implicitly also know the imaginary part through the KK relations

## CLASSICAL MICROSCOPIC THEORY FOR THE ELECTROMAGNETIC RESPONSE OF MATERIALS

In a non-conductive medium, the electrons are localised, i.e. bound to a nucleus or in a bond between two nuclei. In an external electromagnetic field, the electrons are displaced a distance  $r$  from its equilibrium position. This leads to a polarisation

$$\bar{P} = -Ne\bar{r}$$

$N$  is the number of electrons per volume. The displacement  $\bar{D}$  is given by

$$\bar{D} = \varepsilon_0 \bar{E} + \bar{P} = \varepsilon_0 \varepsilon_r \bar{E}$$

According to the classical Lorentz model, the electrons are bound by a force with a linear

force constant  $k$ . The equation of motion is then given by

$$m \frac{d^2 \bar{r}}{dt^2} + m\gamma \frac{d\bar{r}}{dt} + k\bar{r} = -e\bar{E} = -e\bar{E}_0 e^{-i\omega t}$$

$\gamma$  is a damping constant  $m$  is the electron mass. A solution of this differential equation is

$$\bar{r} = \frac{-e\bar{E}_0}{-m\omega^2 - i\omega\gamma + k} e^{-i\omega t}$$

which gives the polarisation  $\bar{P}$

$$\bar{P} = \frac{Ne^2 / m}{-\omega^2 - i\omega\gamma + k / m} \bar{E}$$

$k/m = \omega_0^2$  gives:

$$\bar{P} = \frac{Ne^2 / m}{-\omega^2 - i\omega\gamma + \omega_0^2} \bar{E}$$

With  $\bar{P} = \alpha \bar{E}$  we can write

$$\bar{D} = \epsilon_0 \bar{E} + \bar{P} = (\epsilon_0 + \alpha) \bar{E} = \epsilon_0 \epsilon_r \bar{E}$$

$$\Rightarrow \epsilon_r = 1 + \frac{\alpha}{\epsilon_0}$$

$\epsilon_r$  is the relative dielectric constant

Inserted in the equation above we get:

$$\epsilon_r = 1 + \frac{Ne^2 / m\epsilon_0}{-\omega^2 - i\omega\gamma + \omega_0^2}$$

$Ne^2/m\epsilon_0$  has the dimension  $\text{sek}^{-2}$ , we call it the plasma frequency squared,  $\omega_p^2$

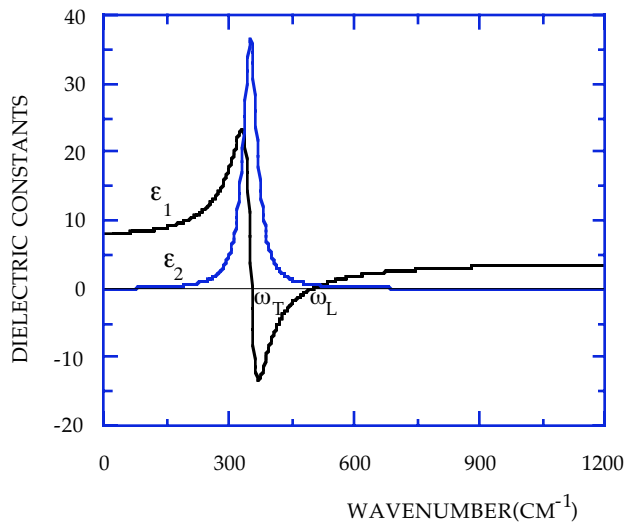
$$\epsilon_r = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma - \omega_0^2} = N^2$$

$\epsilon_r = N^2$  is the dielectric constant of the system It is complex for a system where we have absorption. If we write it out as real and imaginary parts, we get: ( $N = n + i\kappa$ )

$$\epsilon_1 = n^2 - \kappa^2 = 1 + \frac{\omega_p^2(\omega_0^2 - \omega^2)}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}$$

$$\epsilon_2 = 2n\kappa = \frac{\omega_p^2 \cdot \gamma\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}$$

The figure shows the real and imaginary parts for  $\epsilon_r$

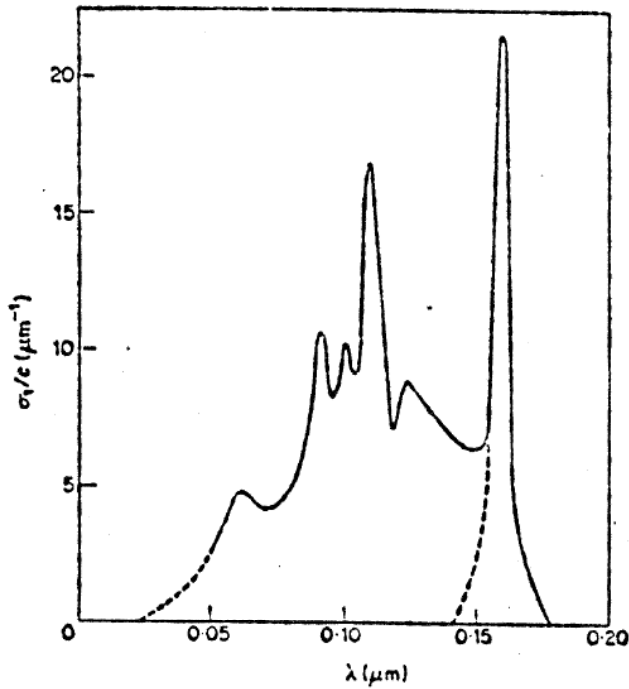


If the system has several resonance frequencies we write:

$$N^2 = \epsilon_r = 1 + \omega_p^2 \sum_j \frac{f_j}{\omega_j^2 - \omega^2 - i\omega\gamma_j}$$

$f_j$  is called the oscillator strength.

In the figure below we show the measure  $\epsilon_2$  or rather  $s=\omega\epsilon_2$  for NaCl. We can see that the spectrum consists of a number of resonances.



One point has been ignored so far.

$$\alpha = \frac{Ne^2 / m}{-\omega^2 - i\omega\gamma + \omega_0^2}$$

should be considered as an atomic polarisability. The field that polarises is the local field, not the external field. This means that  $P/E$  for a crystal is given by

$$P/E = \frac{N\alpha}{1 - \frac{\epsilon_0}{3}\alpha N} = \frac{\epsilon - 1}{\epsilon_0}$$

This can again be considered as an effective polarisability, the atomic get a correction from the fields from the neighbouring atoms in a crystal:

$$\alpha_{eff} = \frac{\alpha}{1 - \frac{\epsilon_0}{3}\alpha N}$$

This can be written in the form (Claussius-Mosottis ligning)

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{\varepsilon_o}{3} \alpha N$$

## DRUDE TEORI FOR METALLER

In metals the electrons are free. This means that  $\omega_0 = 0$  in the equations we derived. Such a theory was first developed by P. DRUDE.

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

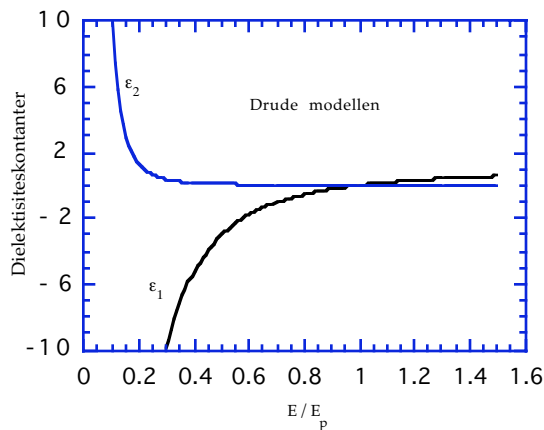
$$\varepsilon_1 = 1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}$$

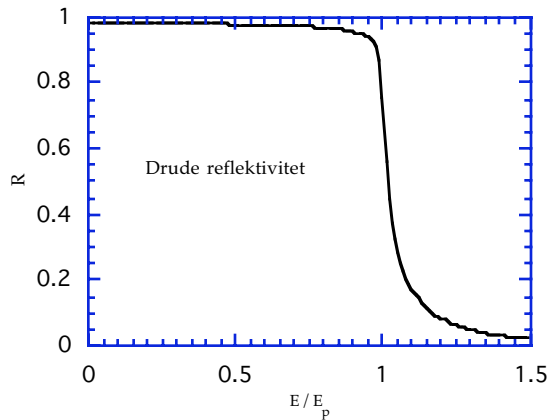
Real part of  $\varepsilon$

$$\varepsilon_2 = \frac{\omega_p^2 \gamma}{\omega(\omega^2 + \gamma^2)}$$

Imaginary part of  $\varepsilon$

$\gamma = 1/\tau$ , where  $\tau$  is the lifetime for excitations in the electron gas, i.e. the time between collisions. Measurements of  $\varepsilon$  allows us to determine the time between collisions in the electron gas. If we plot the equations above:





The same collision time  $\tau$  enters in the expression for the dc conductivity

$$\sigma = Ne^2\tau/m$$

From Maxwells equations

$$\nabla \times \bar{H} = \epsilon_0 \frac{\partial \bar{E}}{\partial t} + \bar{J} = \epsilon_0 \epsilon_r \frac{\partial \bar{E}}{\partial t} + \bar{J} = \frac{\partial \bar{D}}{\partial t}$$

we see that the dielectric constant  $\epsilon_r$  can be written as:

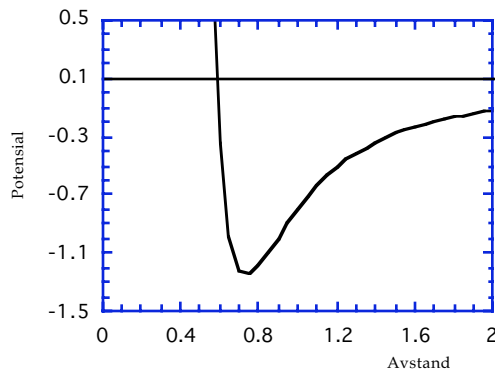
$$\epsilon_r = 1 + i\sigma/\omega\epsilon_0.$$

or  $\epsilon_r = \epsilon_b + i\sigma/\omega\epsilon_0$  if we have both bound and free electrons

## 2. ORDENS PROSESSER

### ANHARMONISK POTENSIAL

WE will now show how second harmonic generation and sum and difference frequency generation follows from a classical oscillator model if we include anharmonic contributions to the potential. We include an anharmonic contribution to the force given by  $\max^2$ . This is the force we get for large amplitude motions around the equilibrium in the potential given by the graph below



Assume that a material is radiated at the same time by two waves. The equation of motion is then, including the anharmonic force

$$m\ddot{x} + \gamma m\dot{x} + kx + max^2 = F = qE_{\text{Tot}}$$

$$\ddot{x} + \gamma\dot{x} + \omega_0^2 x + ax^2 = \frac{q}{m} (E_1(e^{i\omega_1 t} + e^{-i\omega_1 t}) + E_2(e^{i\omega_2 t} + e^{-i\omega_2 t}))$$

If we assume that  $a$  is small we can solve this equation by iteration

$$x = x^{(1)} + x^{(2)} + x^{(3)} \dots$$

$$P = Nq \cdot x$$

The first order solution is found by setting  $a=0$

$$x^{(1)} = \sum_i x^{(1)}(\omega_i) = \sum_i \frac{q/m E_i}{\omega_0^2 - \omega_i^2 - i\omega_i \gamma} e^{\pm i\omega_i t}$$

The second order solution is found by shifting  $(ax^{(1)})^2$  to the right side and insert the first order solution. This gives

$$\ddot{x} + \gamma\dot{x} + \omega_0^2 x = \frac{q}{m} (E_1(e^{i\omega_1 t} + e^{-i\omega_1 t}) + E_2(e^{i\omega_2 t} + e^{-i\omega_2 t})) - a(x^{(1)})^2$$

This is as an ordinary oscillator, but with a new driving force that contains new driving frequencies.  $ax^{(1)}$  is of the form:

$$x^{(1)} = \alpha_1 e^{i\omega_1 t} + \alpha_2 e^{-i\omega_1 t} + \alpha_3 e^{i\omega_2 t} + \alpha_4 e^{-i\omega_2 t}$$

$$\begin{aligned}
(x^{(1)})^2 &= (\alpha_1 e^{i\omega_1 t} + \alpha_2 e^{-i\omega_1 t} + \alpha_3 e^{i\omega_2 t} + \alpha_4 e^{-i\omega_2 t})^2 \\
&= \alpha_1^2 e^{2i\omega_1 t} + \alpha_2^2 e^{-2i\omega_1 t} + \alpha_3^2 e^{2i\omega_2 t} + \alpha_4^2 e^{-2i\omega_2 t} \\
&\quad + \alpha_1 \alpha_3 e^{i(\omega_1 + \omega_2)t} + \alpha_1 \alpha_4 e^{i(\omega_1 - \omega_2)t} \dots \\
&\quad + \alpha_1 \alpha_2 e^{i0 \cdot t} + \dots
\end{aligned}$$

$$\begin{aligned}
\Rightarrow x^{(2)} &= x^{(2)}(\omega_1 + \omega_2) + x^{(2)}(\omega_1 - \omega_2) \\
&+ x^{(2)}(2\omega_1) + x^{(2)}(2\omega_2) + x^{(2)}(0) + \text{c.c.}
\end{aligned}$$

$$\begin{aligned}
\Rightarrow x^{(2)}(\omega_1 \pm \omega_2) &= \frac{2a(q/m)^2 E_1 E_2}{(\omega_0^2 - \omega_1^2 - i\omega_1 \gamma)(\omega_0^2 - \omega_2^2 \mp i\omega_2 \gamma)} \\
&\quad \cdot \frac{1}{\omega_0^2 - (\omega_1 \pm \omega_2)^2 - i(\omega_1 \pm \omega_2)\gamma} \cdot e^{-i(\omega_1 \pm \omega_2)t} \\
x^{(2)}(2\omega_1) &= \frac{-a(q/m)^2 E_1^2 \cdot e^{-2i\omega_1 t}}{(\omega_0^2 - \omega_1^2 - i\omega_1 \gamma)^2 (\omega_0^2 - 4\omega_1^2 - i2\omega_1 \gamma)}
\end{aligned}$$

We see that the systems now oscillates, not only at the frequencies  $\omega_1$  and  $\omega_2$ , but also at  $2\omega_1$ ,  $2\omega_2$ ,  $\omega_1 + \omega_2$ , and  $\omega_1 - \omega_2$ . This is used extensively in laser technology to create lasers at new frequencies.