F8150, 2024

# **Simplest microscopic models**

v. 2.10.2024

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• Revision of classical mechanics (vibrations and waves). Revision of fundamentals of the interaction of electromagnetic waves with matter in quantum mechanics, esp. that with isolated atoms.

• Classical models (Lorentzian oscillator and Drude response of free carriers) are very helpful and instructive. They also allow a specification of the link of microscopic and averaged quantities.

• The simples quantum models are based on perturbation theory. They form a convenient framework for understanding response functions related to one-electron picture of (direct and indirect) transitions of valence electrons in crystals.

## **Lorentzian oscillator**

Charges bound elastically to their equilibrium positions are dislocated by the electrical force of the electromagnetic wave (the magnetic component is negligible). In a harmonic wave travelling along *z,* the wavelength is supposed to be large compared to the spatial structure of the investigated charges; the relevant quantity is then the displacement *r* of the charge *e* in the plane perpendicular to *z*. The force is proportional to the intensity of the electric field of the wave, **lator**<br>tically to their equilibrium positive (the magnetic component is r<br>upposed to be large compared to<br>then the displacement *r* of the clintensity of the electric field of t<br>,  $t$ ) =  $\vec{E}_o e^{i(k_z z - \omega t)}$ .<br>n of motion **i** elastically to their equilibrium position<br> *i* c wave (the magnetic component is negrely is supposed to be large compared to the<br> *i* ity is then the displacement r of the change of the electric field of the<br> *i* the cillator<br>
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imposed to be large compared to the spatia ir equilibrium positions are dislocated by the electrical force of the<br>etic component is negligible). In a harmonic wave travelling along z,<br>elarge compared to the spatial structure of the investigated charges; the<br>blacem

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\vec{E}(z,t) = \vec{E}_o e^{i(k_z z - \omega t)} \quad .
$$

Newtonian equation of motion for the displacement of damped harmonic oscillator of the mass *m* at an arbitrary position *z*:

$$
m\frac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} = -m\omega_o^2\vec{r} - \frac{m}{\tau}\frac{\mathrm{d}\vec{r}}{\mathrm{d}t} - e\vec{E}_o e^{-i\omega t} .
$$

Neglecting the contribution of possible vibrations at the eigenfrequency  $\omega_{o}$ , which is small at times long compared to  $\tau$ , the solution is a harmonic movement with the frequency  $\omega$ ,

$$
\vec{r} = -\frac{e}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} \vec{E}_o e^{-i\omega t} .
$$

The complex values of intensity lead to complex values of the displacement (they have magnitude and *phase*).

The displacement of the charge produces the dipole moment

\n The current of the charge produces the dipole moment\n 
$$
\vec{p} = -e\vec{r} = \alpha \vec{E}, \quad \alpha = \frac{e^2}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}},
$$
\n

\n\n The current of the electric field;  $\alpha$  is called electrical polarizability. It disappears for  $z$  is the electric field;  $\alpha$  is called the electric field polarizability. It disappears for  $z$  is the electric field;  $\alpha$  is the oscillator.\n

\n\n The frequency dependence exhibit the eigenfrequency of the oscillator.\n

\n\n The current of the velocity of the dipole moment (polarization is in a unit volume, the volume density of the dipole moment (polarization is  $\vec{P} = N\vec{p} = N\alpha \vec{E} = \chi \varepsilon_o \vec{E}$ ;\n

\n\n The time of the direction of the magnetic field. The mass is characterized as the temperature of the external field. The ensemble of oscillators is characterized.\n

\n\n The current of the velocity is the magnetic field,  $\chi = \frac{Ne^2}{\varepsilon_o m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}}.$ \n

\n\n The current of the velocity is the electric field,  $\alpha$  is the electric field,  $\alpha$  is the electric field. The energy is the magnetic field,  $\alpha$  is the electric field,  $\alpha$  is the electric field. The energy is the magnetic field,  $\vec{P} = N\vec{p} = N\vec{p}$  is the electric field.\n

proportional to the electric field;  $\alpha$  is called electrical polarizability. It disappears for zero charge (no dipole moment) and infinite mass (no displacement). The frequency dependence exhibits a resonance close to the eigenfrequency of the oscillator.

With *N* oscillators in a unit volume, the volume density of the dipole moment (polarization) is

$$
\vec{P} = N\vec{p} = N\alpha \vec{E} \equiv \chi \varepsilon_o \vec{E} ;
$$

charge produces the dipole moment<br>  $\alpha \vec{E}$ ,  $\alpha = \frac{e^2}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}}$ ,<br>
ric field;  $\alpha$  is called electrical polarizability. It disappears for zero charge (no<br>
nite mass (no displacement). The frequency de the dipole moment<br>  $\frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}}$ ,<br>
End electrical polarizability. It disappears for zero charge (no<br>
blacement). The frequency dependence exhibits a resonance<br>
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blume density of the dipole moment (polari ment of the charge produces the dipole moment<br>  $=-e\vec{r} = \alpha \vec{E}$ ,  $\alpha = \frac{e^2}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}}$ ,<br>
o the electric field;  $\alpha$  is called electrical polarizability. It disappears for zero charge (no<br>
nt) and infini lipole moment<br>  $\frac{1}{-\omega^2 - i \frac{\omega}{\tau}}$ ,<br>
ectrical polarizability. It disappears for zero charge (no<br>
ment). The frequency dependence exhibits a resonance<br>
e density of the dipole moment (polarization) is<br>
the dimensionless it is proportional to the intensity of the wave; the dimensionless coefficient (note the presence of the vacuum permittivity, SI units)  $\chi$  is called susceptibility ("vaspriimčivost" in Russian – the ability to accept the influence of the external field). The ensemble of oscillators is characterized by ment of the charge produces the dipole moment<br>  $=-e\vec{r} = \alpha \vec{E}$ ,  $\alpha = \frac{e^2}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}}$ ,<br>
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called electrical polarizability. It disappears for zero charge (no<br>
o displacement). The frequency dependence exhibits a resonance<br>
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the volume density of the dipole m

$$
\chi = \frac{Ne^2}{\varepsilon_o m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}}.
$$

The SI unit of polarization is  $C/m^2$ , the same as that of area density of charge, or of the electric displacement *D*.

Dielectric function is dimensionless proportionality factor between the electric displacement and field intensity:

$$
\vec{D} = \varepsilon \varepsilon_o \vec{E} = \varepsilon_o \vec{E} + \vec{P} = \varepsilon_o (1 + \chi) \vec{E} \quad \rightarrow \quad \varepsilon = 1 + \chi \quad .
$$

It represents the susceptibility added to to unity (the vacuum contribution to the electric displacement). The ensemble of charged oscillators with the same eigenfrequency and volume density *N* leads to

electric function is dimensionless proportionality factor between the electric displacement a  
\nensity:  
\n
$$
\vec{D} = \varepsilon \varepsilon_o \vec{E} = \varepsilon_o \vec{E} + \vec{P} = \varepsilon_o (1 + \chi) \vec{E} \rightarrow \varepsilon = 1 + \chi .
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\varepsilon = 1 + \chi .
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\varepsilon = \text{ensemble of charged oscillators with the same eigenfrequency and volume density } N \text{ leads}
$$
\n
$$
\varepsilon = 1 + \frac{Ne^2}{\varepsilon_o m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} = 1 + \frac{S\omega_o^2}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} , \text{ where } S = \frac{Ne^2}{\omega_o^2 \varepsilon_o m} .
$$
\n
$$
\varepsilon = S \text{ is dimensionless "oscillator strength", determining the "magnitude of the spectral strua's a further simple meaning, as it is equal to the contribution of the oscillators to static permit\nelectric function at zero frequency). The eigenfrequency of oscillators determines the "spec-\nsition" and the damping time  $\tau$  determines the "spectral width".  
\ne usual notation for the real and imaginary part of the dielectric function uses subscripts 1 a  
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$$
\varepsilon = \varepsilon_1 + i\varepsilon_2 .
$$
$$

*c* function is dimensionless proportionality factor between the electric displacement and field<br>  $\epsilon \varepsilon_o \vec{E} = \varepsilon_o \vec{E} + \vec{P} = \varepsilon_o (1 + \chi) \vec{E} \rightarrow \varepsilon = 1 + \chi$ .<br>
ents the susceptibility added to to unity (the vacuum contri Here, *S* is dimensionless "oscillator strength", determining the "magnitude of the spectral structure"; it has a further simple meaning, as it is equal to the contribution of the oscillators to static permittivity (dielectric function at zero frequency). The eigenfrequency of oscillators determines the "spectral position" and the damping time  $\tau$  determines the "spectral width". ion is dimensionless proportionality factor between the electric displacement an  $\vec{E} = \varepsilon_o \vec{E} + \vec{P} = \varepsilon_o (1+\chi)\vec{E} \rightarrow \varepsilon = 1+\chi$ .<br>
susceptibility added to to unity (the vacuum contribution to the electric displacement ic function is dimensionless proportionality factor between the electric displacement and fi<br>  $y$ :<br>  $= \varepsilon \varepsilon_{\nu} \vec{E} = \varepsilon_{\nu} \vec{E} + \vec{P} = \varepsilon_{o} (1 + \chi) \vec{E} \rightarrow \varepsilon = 1 + \chi$ .<br>
Sents the susceptibility added to to unity (the ction is dimensionless proportionality factor between the electric displacement ar<br>  $\sum_{o} \vec{E} = \varepsilon_{o} \vec{E} + \vec{P} = \varepsilon_{o} (1+\chi)\vec{E} \rightarrow \varepsilon = 1+\chi$ .<br>
the susceptibility added to to unity (the vacuum contribution to the elect nnetion is dimensionless proportionality factor between the electric displacement and fiels<br>  $x_p \vec{E} = x_o \vec{E} + \vec{P} = x_o (1 + \chi)\vec{E} \rightarrow x = 1 + \chi$ ,<br>
the susceptibility added to to unity (the vacuum contribution to the electric di trion is dimensionless proportionality factor between the electric displacement and field<br>  $\vec{E} = \vec{E}_\phi \vec{E} + \vec{P} = \vec{E}_\phi (1 + \chi) \vec{E} \rightarrow \vec{E} = 1 + \chi$ .<br>  $\vec{E} = \vec{E}_\phi \vec{E} + \vec{P} = \vec{E}_\phi (1 + \chi) \vec{E} \rightarrow \vec{E} = 1 + \chi$ .<br>  $\vec{E} = \$ nnetion is dimensionless proportionality factor between the electric displacement and field<br>  $\delta \varepsilon_{\rho} \vec{E} = \varepsilon_{\rho} \vec{E} + \vec{P} = \varepsilon_{o} (1 + \chi) \vec{E} \rightarrow \varepsilon = 1 + \chi$ .<br>
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dded to to unity (the vacuum contribution to the electric displacement).<br>
tors with the same eigenfrequency and vo etric function is dimensionless proportionality factor between the electric displacement and field<br>digy:<br>  $\vec{D} = \varepsilon \varepsilon_o \vec{E} + \vec{P} = \varepsilon_o (1 + \chi) \vec{E} \rightarrow \varepsilon = 1 + \chi$ .<br>
resents the susceptibility added to to unity (the vac dimensionless proportionality factor between the electric displacement and field<br>  $a_{\rho} \vec{E} + \vec{P} = \varepsilon_o (1 + \chi) \vec{E} \rightarrow \varepsilon = 1 + \chi$ .<br>
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s the susceptibility added to to unity (the vacuum contribution to the electric dis<br>
ble of charged oscillators with the same eigenfrequency and volume density N le<br>

The usual notation for the real and imaginary part of the dielectric function uses subscripts 1 and 2:

$$
\varepsilon = \varepsilon_1 + i\varepsilon_2
$$

In the complex plane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the roots of the denominator): equencies, the dielectric function of Lorentzian oscillators has two poles (the<br>  $\frac{S\omega_o^2}{\omega - \omega_1)(\omega - \omega_2}$ ,<br>  $\frac{S\omega_o^2}{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>
on approximate result fro the Lorentzia encies, the dielectric function of Lorentzian oscillators has two poles (the<br>  $\frac{S\omega_o^2}{-\omega_1)(\omega - \omega_2}$ ,<br>  $-\frac{1}{4\tau^2}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>
approximate result fro the Lorentzian spectral profile in cas

$$
\varepsilon = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)},
$$

complex plane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the  
the denominator):  

$$
\mathcal{E} = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)},
$$

$$
\omega_1 = -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}, \quad \omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}.
$$
  
m leads to a common approximate result for the Lorentzian spectral profile in case of the weak  
*z*. Namely, for

This form leads to a common approximate result fro the Lorentzian spectral profile in case of the weak damping. Namely, for

quencies, the dielectric function of Lorentzian of<br>  $S\omega_o^2$ <br>  $\omega - \omega_1)(\omega - \omega_2)$ ,<br>  $\frac{1}{2} - \frac{1}{4\tau^2}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>  $\omega_1$  on approximate result fro the Lorentzian spectral<br>
proximation can be aplex plane of frequencies, the dielectric function of Lorentzian oscillator<br>  $\varepsilon = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\varepsilon = -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>
leads to a common approximate ies, the dielectric function of Lorentzian oscillators has ty<br>  $\frac{S\omega_o^2}{\omega_1\lambda(\omega - \omega_2)}$ ,<br>  $\frac{1}{\tau^2}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>
proximate result fro the Lorentzian spectral profile in case<br>
nation can be Identical differences, the dielectric function of Lorentzian oscillators has<br>
minator):<br>  $\varepsilon = 1 - \frac{5\omega_0^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\frac{i}{2\tau} + \sqrt{\omega_0^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_0^2 - \frac{1}{4\tau^2}}$ .<br>  $\omega_3$  a common appr ane of frequencies, the dielectric function of Lo<br>
innator):<br>  $\therefore$  = 1 -  $\frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{2\tau}}$ <br>
a common approximate result fro the Lorentzi<br>
fo omplex plane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the<br>
the denominator):<br>  $\varepsilon = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\omega_i = -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1$ ane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the<br>
inator):<br>  $= 1 - \frac{S\omega_0^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\frac{i}{\tau} + \sqrt{\omega_0^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_0^2 - \frac{1}{4\tau^2}}$ .<br>
a a common ap lex plane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the<br>denominator):<br> $\varepsilon = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br> $= -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>ead  $\frac{2}{2}$  - 1 +  $\frac{S\omega_o}{\omega}$   $\frac{\omega_o - \omega}{\omega_o + i \frac{S\omega_o}{\omega}}$   $\frac{\overline{2\tau}}{\sqrt{2\tau}}$ on of Lorentzian oscillators has two poles (<br>  $-\sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>
Lorentzian spectral profile in case of the we<br>
1 as<br>  $\frac{\omega}{2} + \frac{1}{4\tau^2} + i\frac{S\omega_o}{2} - \frac{\frac{1}{2\tau}}{(\omega_o - \omega)^2 + \frac{1}{4\tau^2}}$ . orentzian oscillators has two poles (the<br>  $\frac{1}{4\tau^2}$ .<br>
ian spectral profile in case of the weak<br>  $\frac{1}{2} + i \frac{S\omega_o}{2} \frac{\frac{1}{2\tau}}{(\omega_o - \omega)^2 + \frac{1}{4\tau^2}}$ . 1 e complex plane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the<br>
of the denominator):<br>  $\mathcal{E} = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\omega_1 = -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt$ dielectric function of Lorentzian oscillators has two poles (the<br>  $\overline{\omega_2}$ )<br>  $\overline{\omega_2} = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ <br>  $\overline{\omega}$  result fro the Lorentzian spectral profile in case of the weak<br>
on be expressed as<br>  $\frac{\omega_o}{$ mplex plane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the<br>
he denominator):<br>  $\varepsilon = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\omega_1 = -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{$ of frequencies, the dielectric function of Lorentzian oscillators ha<br> *oor*):<br>  $1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>
(open on approximate result fro the Lorentzian ex plane of frequencies, the dielectric function of Lorentzian oscillators has two<br>
denominator):<br>  $\varepsilon = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $= -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ .<br>
Ads to a co  $\mathcal{E} \approx 1 - \frac{1}{2\pi\left(\frac{1}{2}\right)} = 1 - \frac{1}{2}$ c of frequencies, the dielectric function of Lorentzian oscillators has two poles (the<br>
nator):<br>  $= 1 - \frac{S\omega_0^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $+ \sqrt{\omega_0^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_0^2 - \frac{1}{4\tau^2}}$ .<br>
common approximate resu plex plane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the<br>
denominator):<br>  $\varepsilon = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $= -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ . Lencies, the dielectric function of Lorentzian oscillators has two poles (the<br>  $\frac{S\omega_0^2}{-\omega_1)(\omega - \omega_2}$ ,  $\omega_2 = -\frac{i}{2\tau} - \sqrt{\omega_0^2 - \frac{1}{4\tau^2}}$ .<br>
approximate result fro the Lorentzian spectral profile in case of the weak the complex plane of frequencies, the dielectric function of Lorentzian oscillators has two poles (the<br>
so of the denominator):<br>  $\varepsilon = 1 - \frac{S\omega_o^2}{(\omega - \omega_1)(\omega - \omega_2)}$ ,<br>  $\omega_1 = -\frac{i}{2\tau} + \sqrt{\omega_o^2 - \frac{1}{4\tau^2}}$ ,  $\omega_2 = -\frac{i}{2\tau} 1 \t 1 \t 1$  $\frac{1}{\tau}$  <<  $\omega_o$ , the approximation can be expressed as  $<<$ 

This approximation can be used only for the frequencies close to the eigenfrequency, due to the following approximation of the poles in the complex plane,

$$
\omega_{1,2} \approx -\frac{i}{2\tau} \pm \omega_o
$$
 and  $\omega - \omega_2 \approx 2\omega_o$ ,

usable for small damping. Within this approximation, the imaginary part of  $\epsilon$  is bell-shaped, symmetric lineshape about the eigenfrequency, with the maximum of on can be used only for the frequencies close to the eigenmation of the poles in the complex plane,<br>  $\theta_{1,2} \approx -\frac{i}{2\tau} \pm \omega_o$  and  $\omega - \omega_2 \approx 2\omega_o$ ,<br>
damping. Within this approximation, the imaginary part<br>
he eigenfrequen mly for the frequencies close to the eights<br>objets in the complex plane,<br> $\omega_o$  and  $\omega - \omega_2 \approx 2\omega_o$ ,<br>of this approximation, the imaginary pacy, with the maximum of<br> $\tau$ .<br>THM) is ion can be used only for the frequencies close to the eigenfrequency, due to the<br>
ximation of the poles in the complex plane,<br>  $\omega_{1,2} \approx -\frac{i}{2\tau} \pm \omega_o$  and  $\omega - \omega_2 \approx 2\omega_o$ ,<br>
1 damping. Within this approximation, the ima an can be used only for the frequencies close to the eigenfrequency, due to the<br>mation of the poles in the complex plane,<br> $\frac{\partial}{\partial z} \approx -\frac{i}{2\tau} \pm \omega_o$  and  $\omega - \omega_2 \approx 2\omega_o$ ,<br>amping. Within this approximation, the imaginary can be used only for the frequencies close to the eigenfrequency, due to<br>tion of the poles in the complex plane,<br> $\approx -\frac{i}{2\tau} \pm \omega_o$  and  $\omega - \omega_2 \approx 2\omega_o$ ,<br>pping. Within this approximation, the imaginary part of  $\varepsilon$  is be

$$
\varepsilon_{2,\max} = S\omega_o \tau
$$

Full width at half-maximum (FWHM) is

$$
\Delta \omega = 1/\tau
$$

Real part is antisymmetric about the eigenfrequency.

Spectral lineshapes on the real axis of frequencies complies with the general requirement

$$
\varepsilon(-\omega) = \varepsilon^*(\omega)
$$

where the asterix denotes complex conjugation.



Dielectric function of Lorentz oscillators (S=4, tau\*omega\_0=5).

An example of the difference between the exact and approximate form of the Lorentzian lineshapes for the real ("dispersive") and imaginary ("absorptive") parts of the dielectric function:



Real (left) and imaginary (right) part of the dielectric function  $(S=4, \tau)$  tau\*omega\_0=5), exact (ex), approximate (aprox) forms and their difference (dif). Relative agreement of the exact and approximate form improves for narrower Lorentzian profiles (longer times  $\tau$ :



Lorentz osc, epsilon 1

Real part of the Lorentzian dielectric function (left:  $S=4$ , tau\*omega\_0=15, right: tau\*omega\_0=50), exact (ex), approximate (aprox), difference (dif).

Refractive index is the square root of the dielectric function. Using the common conventions:

$$
N = n + ik \, , \, n = \sqrt{(\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2})/2} \, , \, k = \sqrt{(-\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2})/2} = \frac{\varepsilon_2}{2n} \, ,
$$

where *n* and *k* are real. The real part (*n*) is always positive, the positive square root is assumed; the sign of *k* is the same as that of the imaginary part of the dielectric function – it describes the damping of the wave, travelling in the opposite direction for negative frequencies.



Complex refractive index of Lorentzian oscillators  $(S=4, \tau)$  tau\*omega\_0=5).

Complex refractive index determines the reflectivity at planar interfaces. Fresnel amplitude reflectance *r* for the normal incidence at the interface with vacuum (the unit refractive index) is

$$
r = \sqrt{R}e^{i\Phi} = (n-1+ik)/(n+1+ik) ,
$$

where  $R$  is the squared modulus of  $r$ , i.e., the power reflectivity.



Normal-incidence reflectivity and the phase angle of *r* (S=4, tau\*omega\_0=5).

The bands of large reflectivity above the eigenfrequency are called "reststrahlen". They become more pronounced esp. for small damping of the oscillators.



Lorentz osc, reststrahlen

Normal-incidence reflectvance (S=4, tau\*omega\_0=5, 15 a 50).

#### Complex conductivity

The velocity of the charge displacement in the Lorentz model is

conductivity  
\nty of the charge displacement in the Lorentz model is  
\n
$$
\frac{d\vec{r}}{dt} = i\omega \frac{e}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} \vec{E}_o e^{-i\omega t}
$$
\nnt density produced by this movement equals to the charge  
\nin the direction of the velocity. Assuming the concentration  
\nproportional to the field intensity, where the proportionality  
\n
$$
iN e \frac{d\vec{r}}{dt} = i\omega \frac{Ne^2}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} \vec{E}_o e^{-i\omega t} \equiv \sigma \vec{E}_o e^{-i\omega t}
$$

The current density produced by this movement equals to the charge transferred through unit area per unit time in the direction of the velocity. Assuming the concentration *N* of the oscillators, the current density is proportional to the field intensity, where the proportionality factor  $\sigma$  is called conductivity: Lorentz n<br> *i ti*<br>
i t equals<br>
ing the the reference by displacement in the Lorentz model is<br>  $\omega_o^2 - \omega^2 - i \frac{\omega}{\tau} \vec{E}_o e^{-i\omega t}$ .<br>
duced by this movement equals to the charge transferred through unit area per<br>
n of the velocity. Assuming the concentration N of the oscillat splacement in the Lorentz model is<br>  $-\omega^2 - i\frac{\omega}{\tau} \vec{E}_o e^{-i\omega t}$ .<br>
d by this movement equals to the charge transferred through unit area per<br>
the velocity. Assuming the concentration N of the oscillators, the current<br>
e model is<br>
s to the charge transfer<br>
e concentration *N* of the<br>
proportionality factor<br>  $i\omega t \equiv \sigma \vec{E}_o e^{-i\omega t}$ .<br>
driving force, which re entz model is<br>  $\cdot$ <br>
quals to the charge transferr<br>
g the concentration *N* of the<br>
the proportionality factor<br>  $\int_{0}^{1} e^{-i\omega t} \equiv \sigma \vec{E}_{0} e^{-i\omega t}$ .<br>
the driving force, which re rge displacement in the Lorentz model is<br>  $\frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} \vec{E}_o e^{-i\omega t}$ .<br>
coluced by this movement equals to the charge transferred through unit area per<br>
of the velocity. Assuming the concentration *N* of the acement in the Lorentz model is<br>  $\frac{1}{\rho^2 - i \frac{\omega}{\tau}} \vec{E}_o e^{-i\omega t}$ .<br>
y this movement equals to the charge transferred through unit area per<br>
velocity. Assuming the concentration *N* of the oscillators, the current<br>
eld i conductivity<br>
city of the charge displacement in the Lorentz model is<br>  $\frac{d\vec{r}}{dt} = i\omega \frac{e}{m} \frac{1}{\omega_s^2 - \omega^2 - i} \frac{\omega}{\tau} \vec{E}_s e^{-i\omega s}$ .<br>
cent density produced by this movement equals to the charge transferred through uni ment in the Lorentz model is<br>  $\frac{1}{t} \frac{\partial}{\partial \theta} \vec{E}_{\phi} e^{-i\omega t}$ .<br>
is movement equals to the charge transferred through unit area per<br>
oricity. Assuming the concentration *N* of the oscillators, the current<br>
ntensity, whe

ex conductivity

\nlocity of the charge displacement in the Lorentz model is

\n
$$
\frac{d\vec{r}}{dt} = i\omega \frac{e}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} \vec{E}_o e^{-i\omega t}
$$
\ncurrent density produced by this movement equals to the charge transferred throw

\ntime in the direction of the velocity. Assuming the concentration *N* of the oscillat

\nby is proportional to the field intensity, where the proportionality factor  $\sigma$  is call

\n
$$
\vec{j} = N e \frac{d\vec{r}}{dt} = i\omega \frac{Ne^2}{m} \frac{1}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} \vec{E}_o e^{-i\omega t} \equiv \sigma \vec{E}_o e^{-i\omega t}
$$
\ncurrent density is usually not in phase with the driving force, which results in

\n
$$
\frac{A/m^2}{V/m} = \frac{1}{\Omega m}
$$

The current density is usually not in phase with the driving force, which results in the complex-valued conductivity. Its SI unit is

$$
\frac{A/m^2}{V/m} = \frac{1}{\Omega m} .
$$

A convenient expression for the conductivity is

venient expression for the conductivity is

\n
$$
\sigma \equiv \sigma_1 + i\sigma_2 = -i\omega \varepsilon_o (\varepsilon - 1) = -i\omega \frac{Ne^2}{m} \frac{1}{\omega_o^2 - \omega^2 - i\frac{\omega}{\tau}}
$$
\n
$$
= -i\omega \frac{S\varepsilon_o \omega_o^2}{\omega_o^2 - \omega^2 - i\frac{\omega}{\tau}} \quad , \text{ where } S = \frac{Ne^2}{\omega_o^2 \varepsilon_o m} \quad .
$$
\nas the dimensionless oscillator strength silu *S*. At the eigenfrequency, the conductivity is real,  $\sigma(\omega_o) = S\varepsilon_o \omega_o^2 \tau$ .

\nis value is convenient in expressing the dimensionless quantity

\n
$$
\frac{\sigma}{\sigma(\omega_o)} = -i \frac{\frac{\omega}{\tau}}{\omega_o^2 - \omega^2 - i\frac{\omega}{\tau}} = \frac{1}{1 + i\omega_o \tau(\omega_o / \omega - \omega / \omega_o)} \quad .
$$
\n15

It uses the dimensionless oscillator strength sílu *S*. At the eigenfrequency, the conductivity is real,

$$
\sigma(\omega_o) = S \varepsilon_o \omega_o^2 \tau .
$$

This value is convenient in expressing the dimensionless quantity

$$
\frac{\sigma}{\sigma(\omega_o)} = -i \frac{\frac{\omega}{\tau}}{\omega_o^2 - \omega^2 - i \frac{\omega}{\tau}} = \frac{1}{1 + i \omega_o \tau(\omega_o / \omega - \omega / \omega_o)}.
$$

The spectral dependence of complex conductivity on real axis is even and odd in its real and imaginary parts, respectively. The real part decays for large frequencies as  $1/\omega^2$ , the imaginary part as  $1/\omega$ .



Lorentz\_osc, sigma

Conductivity of Lorentz oscillators (S=4, tau\*omega\_0=5).

### **Drude model for free charge carriers**

The elastic bonding of charges to their equilibrium positions might disappear (e.g., for electrons in metals, or electrons and holes in semiconductors). This corresponds to the vanishing eigenfrequency of the Lorentzian oscillator. The displacement and velocity of the free charge carriers are

$$
\vec{r} = \frac{e}{m} \frac{1}{\omega(\omega + i/\tau)} \vec{E}_o e^{-i\omega t} \ , \ \ \frac{\mathrm{d}}{\mathrm{d}t} \vec{r} = -i \frac{e}{m} \frac{1}{(\omega + i/\tau)} \vec{E}_o e^{-i\omega t} \ .
$$

Using the carrier density *N* and their mass *m*, we arrive at the dielectric function

**ude model for free charge carriers**  
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Lorentzian oscillator. The displacement and velocity of the free charge carriers are  

$$
\vec{r} = \frac{e}{m} \frac{1}{\omega(\omega + i/\tau)} \vec{E}_e e^{-i\omega t}, \quad \frac{d}{dt} \vec{r} = -i \frac{e}{m} \frac{1}{(\omega + i/\tau)} \vec{E}_e e^{-i\omega t}
$$
ing the carrier density *N* and their mass *m*, we arrive at the dielectric function  

$$
\varepsilon = 1 - \frac{Ne^2}{\varepsilon_e m} \frac{1}{\omega(\omega + i \frac{1}{\tau})} = 1 - \frac{\omega_p^2}{\omega^2 + \frac{1}{\tau^2}} + i \frac{\tau}{\omega(\omega^2 + \frac{1}{\tau^2})}, \text{ where } \omega_p = \sqrt{\frac{Ne^2}{\varepsilon_e m}}.
$$
The oscillator strength of the Lorentz formula is replaced by the square of plasma frequency; the name  
avokes the possibility of collective vibrations in the plasma of free carriers at this frequency.  
IB: setting the eigenfrequency of the Lorentzian oscillator to zero provides an approximation of its  
ehaviour for large frequencies, with the motion independent of the elastic bonds.

The oscillator strength of the Lorentz formula is replaced by the square of *plasma frequency*; the name invokes the possibility of collective vibrations in the plasma of free carriers at this frequency.

NB: setting the eigenfrequency of the Lorentzian oscillator to zero provides an approximation of its behavior for large frequencies, with the motion independent of the elastic bonds.

The two poles of the Drude dielectric function are:

$$
\omega_1 = 0 \quad \text{a} \quad \omega_2 = -\frac{i}{\tau} \quad .
$$

As the modulus of complex frequency increases, the dielectric function approaches unity fast enough to warrant the unimportance of the pole at the origin in deriving the Kramers-Kronig relation of the Drude dielectric function are:<br>  $D_1 = 0$  a  $\omega_2 = -\frac{i}{\tau}$ .<br>
In so f complex frequency increases, the importance of the pole at the origin es of the Drude dielectric function are:<br>  $\omega_1 = 0$  a  $\omega_2 = -\frac{i}{\tau}$ .<br>
Ilus of complex frequency increases, the dielectric function approaches unity fast enough to unimportance of the pole at the origin in deriving the K f the Drude dielectric function are:<br>
= 0 a  $\omega_2 = -\frac{i}{\tau}$ .<br>
of complex frequency increases, the dielectric function approaches unity fast enough to<br>
aportance of the pole at the origin in deriving the Kramers-Kronig rel

poles of the Drude dielectric function are:  
\n
$$
\omega_1 = 0
$$
 a  $\omega_2 = -\frac{i}{\tau}$   
\nnodulus of complex frequency increases, the  
\nthe unimportance of the pole at the origin in  
\n $\varepsilon_2(\omega) = -\frac{2\omega}{\pi} \int_0^\infty \frac{\varepsilon_1(\Omega) - 1}{\Omega^2 - \omega^2} d\Omega$   
\npart is on real axis is even, the imaginary p  
\nreasing frequency, the real part is growing  
\n $\varepsilon_1(0) = 1 - (\omega_p \tau)^2$ 

The real part is on real axis is even, the imaginary part odd. With increasing frequency, the real part is growing monotonically from

$$
\varepsilon_1(0) = 1 - (\omega_p \tau)^2
$$

bles of the Drude dielectric function are:<br>  $\omega_1 = 0$  a  $\omega_2 = -\frac{i}{\tau}$ .<br>
thulus of complex frequency increases, the dielectric<br>
unimportance of the pole at the origin in deriving<br>  $(\omega) = -\frac{2\omega}{\pi} \int_0^{\infty} \frac{\varepsilon_1(\Omega) - 1}{$ poles of the Drude dielectric function are:<br>  $\omega_1 = 0$  a  $\omega_2 = -\frac{i}{\tau}$ .<br>
andulus of complex frequency increases, the dielectric function approaches unity fast enough to<br>
the unimportance of the pole at the origin in der Drude dielectric function are:<br>
a  $ω_2 = -\frac{i}{\tau}$ <br>
mplex frequency increases, the dielectric function approaches unity fast enough to<br>
mee of the pole at the origin in deriving the Kramers-Kronig relation<br>  $\frac{2ω}{\pi} \int_0$ or the Drude dielectric function are:<br>
= 0 a  $ω_2 = -\frac{i}{\tau}$ .<br>
of complex frequency increases, the dielectric function approaches unity fast enough to<br>
apportance of the pole at the origin in deriving the Kramers-Kronig de dielectric function are:<br>  $ω_2 = -\frac{i}{\tau}$ .<br>
ex frequency increases, the dielectric function approaches unity fast enough to<br>
of the pole at the origin in deriving the Kramers-Kronig relation<br>  $\int_0^\infty \frac{\mathcal{E}_1(\Omega) - 1}{\Omega$ oles of the Drude dielectric funct<br>  $\omega_1 = 0$  a  $\omega_2 = -\frac{i}{\tau}$ .<br>
dulus of complex frequency incre<br>
e unimportance of the pole at the<br>  $\mu(\omega) = -\frac{2\omega}{\pi} \int_0^\infty \frac{\varepsilon_1(\Omega) - 1}{\Omega^2 - \omega^2} d\Omega$ <br>
ant is on real axis is even, t poles of the Drude dielectric function are:<br>  $\omega_1 = 0$  a  $\omega_2 = -\frac{i}{\tau}$ .<br> **odulus of complex frequency increases, the dielectric function approaches unity fast enough to<br>
be unimportance of the pole at the origin in deri** towards unity (the response of vacuum, as the charges are not able to follow the fast changes of the electromagnetic field); the imaginary part is singular at zero, and approaches zero as the inverse third power of frequency.

Note, in particular, the behavior of the real part (esp. the zero crossing close to the plasma frequency):



Drude, epsilon

Dielectric function of the Drude model (omega\_p=1, tau=10). Above 0.75, both parts are multiplied by 100.

Negative inverse of the dielectric function,

rse of the dielectric function,

\n
$$
-\frac{1}{\varepsilon} = \frac{\omega^2 + i\frac{\omega}{\tau}}{\omega_p^2 - \omega^2 - i\frac{\omega}{\tau}}
$$
\nn a narrow neighborhood of the plasma frequency) th

\nIt is proportional to the absorbed energy of longitudinal

ressembles (in a narrow neighborhood of the plasma frequency) the resonance of the Lorentz model. Its imaginary part is proportional to the absorbed energy of longitudinal waves, observable by the EELS technique (Electron Energy Loss Spectroscopy). Note the simple relation: e dielectric function,<br>  $\omega^2 + i \frac{\omega}{\tau}$ <br>  $\omega_p^2 - \omega^2 - i \frac{\omega}{\tau}$ ,<br>
ow neighborhood of the plasma frequency) the resonance of the Lorentz model. Its<br>
portional to the absorbed energy of longitudinal waves, observable by th rse of the dielectric function,<br>  $-\frac{1}{\varepsilon} = \frac{\omega^2 + i\frac{\omega}{\tau}}{\omega_p^2 - \omega^2 - i\frac{\omega}{\tau}}$ ,<br>
n a narrow neighborhood of the plasma frequency) the resonance of the Lorentz model. Its<br>
n is proportional to the absorbed energy of lo electric function,<br>  $\frac{\partial^2 + i \frac{\omega}{\tau}}{\tau}$ <br>  $-\omega^2 - i \frac{\omega}{\tau}$ ,<br>
heighborhood of the plasma frequency) the resonance of the Lorentz model. Its<br>
sional to the absorbed energy of longitudinal waves, observable by the EELS<br>
gy f the dielectric function,<br>  $\omega^2 + i \frac{\omega}{\tau}$ <br>  $= \frac{\omega^2 + i \frac{\omega}{\tau}}{\omega_{\rho}^2 - \omega^2 - i \frac{\omega}{\tau}}$ ,<br>
arrow neighborhood of the plasma frequency) the resonance of the Lorentz model. Its<br>
arrow neighborhood of the plasma frequency) t se of the dielectric function,<br>  $-\frac{1}{\varepsilon} = \frac{\omega^2 + i \frac{\omega}{\varepsilon}}{\omega_p^2 - \omega^2 - i \frac{\omega}{\tau}}$ ,<br>
n a narrow neighborhood of the plasma frequency) the resonance of the Lorentz model. Its<br>
t is proportional to the absorbed energy of l

$$
-\frac{1}{\varepsilon}(\omega_p) = -1 + i\omega_p \tau
$$

The resonance at the plasma frequency has a nearly Lorentzian profile:



Drude, -InvEpsilon

Negative inverse of the Drude dielectric function (tau\*omega\_p=10).

Conductivity is the convenient response function of free carriers; in the Drude model,

ductivity is the convenient response function of free carriers; in the Drude model,  
\n
$$
\sigma \equiv \sigma_1 + i\sigma_2 = -i\omega\varepsilon_o(\varepsilon - 1) = -i\varepsilon_o \frac{\omega_p^2 \tau}{\omega \tau + i}
$$
\n
$$
= \sigma_o \left( \frac{1}{(\omega \tau)^2 + 1} + i \frac{\omega \tau}{(\omega \tau)^2 + 1} \right), \text{ where } \sigma_o = \varepsilon_o \omega_p^2 \tau = \frac{Ne^2 \tau}{m}.
$$
\nexpected, the dc conductivity is proportional to the damping time constant, and inversely  
\nproportional to the mass. The frequency dependence depends solely on the damping time.  
\nsoorbed energy is proportional to the real part (cf. with the Joule heat *U*<sup>7</sup>/*R* developed with the dc  
\ntange *U* on the resistance *R*).  
\ne simple frequency dependence of the absorptive (real) part allows for a direct check of the (general)  
\nn rule  
\n
$$
\frac{2}{\pi\varepsilon_o} \int_0^\infty \sigma_1(\Omega) d\Omega = \omega_p^2.
$$
\nen the carrier concentration stays constant, possible changes in the frequency dependence of the  
\norption processes are limited by the constant area below the real part of conductivity.

As expected, the dc conductivity is proportional to the damping time constant, and inversely proportional to the mass. The frequency dependence depends solely on the damping time. Absorbed energy is proportional to the real part (cf. with the Joule heat  $U^2/R$  developed with the dc voltage *U* on the resistance *R*). of free carriers; in the Drude model,<br>  $\frac{\omega_p^2 \tau}{\nu \tau + i}$ <br>
ere  $\sigma_o = \varepsilon_o \omega_p^2 \tau = \frac{Ne^2 \tau}{m}$ .<br>
to the damping time constant, and inversely<br>
lence depends solely on the damping time.<br>
(cf. with the Joule heat  $U^2/R$  deve

The simple frequency dependence of the absorptive (real) part allows for a direct check of the (general) sum rule

$$
\frac{2}{\pi \varepsilon_o} \int_0^\infty \sigma_1(\Omega) d\Omega = \omega_p^2.
$$

When the carrier concentration stays constant, possible changes in the frequency dependence of the absorption processes are limited by the constant area below the real part of conductivity.

Spectral dependence of the complex conductivity has an even real, and odd imaginary part. The real part decays as  $1/\omega^2$ , the imaginary part as  $1/\omega$ , for high frequencies.



Drude, sigma

Complex conductivity of the Drude model (tau\*omega\_p=10).

Both parts of the refractive index diverge with the frequency approaching zero, due to the divergence of the imaginary part of the dielectric function:

$$
N = n + ik , \quad n = \sqrt{(\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2})/2} , \quad k = \sqrt{(-\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2})/2} = \frac{\varepsilon_2}{2n} ,
$$



Similar to the Lorentz model is the band of high reflectivity at the normal incidence; here it starts at the zero frequency:



Normal-incidence reflectance and the phase of amplitude reflectance of the Drude model (tau\*omega\_p=10).

The large values of the reflectivity below the plasma frequency are the consequence of different importance of the closeness of the numerator and denominator in

$$
R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}
$$
, namely  $n \ll 1$ , or  $k \gg n$ , or  $n \gg 1$ .

For weak damping, the normal-incidence reflectance is only weakly dependent on  $\tau$ .



Normal-incidence reflectance of the Drude model (tau\*omega\_p=3, 30, and 300).

Travelling plane wave looses its amplitude in the direction of propagation (*z*), whenever the imaginary part of the refractive index is nonzero. The decrease of the amplitude is exponential, characterized by the "penetration depth of light". It results from the square of wavenumber, soses its amplitude in<br>ex is nonzero. The de-<br>ht". It results from the<br> $(\omega) \frac{\omega^2}{c^2}$ ,<br>city in vacuum. The am we looses its amplitude in the direction of propagation (*z*), whenever the imaginary<br>index is nonzero. The decrease of the amplitude is exponential, characterized by the<br>f light". It results from the square of wavenumber

$$
k_z^2 = \varepsilon(\omega) \frac{\omega^2}{c^2} ,
$$

where *c* is the light velocity in vacuum. The amplitude is diminished by  $1/e$  of the initial value (about 37%) on the distance

$$
\delta_z = \frac{1}{\text{Im}\left\{k_z\right\}} = \frac{c}{k\omega} ,
$$

boses its amplitude in the direction<br>
ex is nonzero. The decrease<br>
ht". It results from the squan<br>  $(\omega) \frac{\omega^2}{c^2}$ ,<br>  $\therefore$ <br>  $\frac{\omega^2}{k_z} = \frac{c}{k\omega}$ ,<br>
part of the refractive index.<br>
cation of 1/k by the vacuum<br>
ance, the i wave looses its amplitude in the direction of propagation (*z*), whenever the imaginary<br>tive index is nonzero. The decrease of the amplitude is exponential, characterized by the<br>th of light". It results from the square of where *k* is the imaginary part of the refractive index. Spectral dependence of the penetration depth results from the multiplication of  $1/k$  by the vacuum wavelength reduced by the factor of  $2\pi$ . When travelling this distance, the intensity is reduced by the factor  $1/e^2$  (about 14%) of its initial value.

In the range of large reflectivity, the penetration dept is small. With the plasma frequency in the midinfrared range, e.g.,

$$
\lambda_{\text{vac}} = 10 \ \mu \text{m}
$$
,  $v_{\text{vac}} = 1000 \text{ cm}^{-1}$ ,  $\hbar \omega = 124 \text{ meV}$ ,

the penetration depth at the half of the plasma frequency is about 3 microns.



Inverse of the imaginary part of refractive index in the Drude model (tau\*omega\_p=3, 10, 30).

The usual term for the penetration length al low frequencies is "skin depth", as the field penetrates into small depths below the surface of conductors. In our model, the relevant quantity is

$$
k_z \approx \frac{1+i}{\sqrt{2}} \frac{\omega_p}{\sqrt{\omega/\tau}} \frac{\omega}{c} \quad \text{for} \quad \omega \ll 1/\tau \quad .
$$

gth al low frequencies is "skin diductors. In our model, the releva<br>
for  $\omega \ll 1/\tau$ .<br>
dex increases towards zero as the<br>
dex increases towards zero as the<br>
creases as its inverse. In the limiterms of the dc conductivity a w frequencies is "skin depth", as the field penetrates into<br>
In our model, the relevant quantity is<br>  $\omega \ll 1/\tau$ ,<br>
reases towards zero as the square root of frequency;<br>
as its inverse. In the limit of small frequencies, th ration length al low frequencies is "skin depth", as the field penetrates into<br>
ce of conductors. In our model, the relevant quantity is<br>  $\frac{\omega_p}{\omega/\tau} \frac{\omega}{c}$  for  $\omega \ll 1/\tau$ .<br>
fractive index increases towards zero as the The usual term for the penetration length al low frequencies is "skin depth", as the field penetrates into<br>
small depths below the surface of conductors. In our model, the relevant quantity is<br>  $k_z \approx \frac{1+i}{\sqrt{2}} \frac{\omega_p}{\sqrt{\omega/\$ consequently, the penetration depth increases as its inverse. In the limit of small frequencies, the penetration depth can be expressed in terms of the dc conductivity as

For the penetration length al low frequencies  
ow the surface of conductors. In our model  

$$
\approx \frac{1+i}{\sqrt{2}} \frac{\omega_p}{\sqrt{\omega/\tau}} \frac{\omega}{c}
$$
 for  $\omega \ll 1/\tau$   
art of the refractive index increases toward  
e penetration depth increases as its inverse.  
h can be expressed in terms of the dc condi  

$$
\delta_z = \frac{1}{\text{Im} \{k_z\}} \approx \sqrt{\frac{2}{\sigma_o \mu_o \omega}},
$$
  
vacuum permeability.  
activity of 10<sup>5</sup> 1/Ohm.cm and the "optical"  
or the "radio" frequency of 100 MHz rough

comprising the vacuum permeability.

etration length al low frequencies is "<br>face of conductors. In our model, the<br> $\frac{\omega_p}{\sqrt{\omega/\tau}} \frac{\omega}{c}$  for  $\omega \ll 1/\tau$ .<br>Therefore index increases towards zer<br>on depth increases as its inverse. In the<br>spressed in terms of the ration length al low frequen<br> *z* o *c* or *conductors. In our mo<br>*  $\frac{\omega_p}{\omega/\tau} \frac{\omega}{c}$  *for*  $\omega \ll 1/\tau$ *<br>
fractive index increases tow<br>
<i>n* depth increases as its inverses of the dc co<br> *k*<sub>z</sub>  $\left.\frac{2}{\sigma_o \mu_o \omega}\right|$ ,<br> *neabil* gth al low frequencies is "skin depth", as the field penetrates into<br>ductors. In our model, the relevant quantity is<br>for  $\omega \ll 1/\tau$ .<br>dex increases towards zero as the square root of frequency;<br>creases as its inverse. In t the penetration length al low frequencies is "skin depth", as the field penetrates into<br>the surface of conductors. In our model, the relevant quantity is<br> $\frac{1+i}{\sqrt{2}} \frac{\omega_p}{\sqrt{\omega/\tau}} \frac{\omega}{c}$  for  $\omega \ll 1/\tau$ .<br>of the refractive For the dc conductivity of  $10^5$  1/Ohm.cm and the "optical" frequency of 1 THz, the penetration depth is about 160 nm, for the "radio" frequency of 100 MHz roughly 16 microns. The common form of the skin depth,

$$
\delta_z = \sqrt{\frac{2\rho}{\mu\omega}} \; ,
$$

contains the resistivity (the inverse of conductivity) and the permeability of the conductor; the latter might differ from the vacuum value at low frequencies.

## **Quantum transitions in perturbation theory**

The light wave is composed by a train of photons, carrying quantized energy. They can be absorbed during the interaction with matter.

In the manybody system of condensed matter, elementary excitations in the form of quasiparticles can be identified (electrons, holes, excitons, phonons etc.).

The photon and quasiparticle fields influence each other via their interactions ("scattering", "collisions"). One of the basic processes is the absorption of a photon, with the transfer of its energy to the quasiparticle system.

Other processes are possible, such as elastic or inelastic scattering of photons, when a photon survives the collision in a modified form (direction of propagation and/or energy). Important processes involve spontaneous or stimulated emission of photons, carrying energy taken from quasiparticles.

In the case of small changes of the studied system, caused by a weak optical field, the prediction of response functions can be based on the standard perturbation theory of quantum mechanics.

A convenient quantity to be calculated is the energy taken from a harmonic electromagnetic wave in a unit volume per unit of time, linked to the imaginary part of the dielectric function,

$$
{\cal Q} = \frac{1}{2} \, \omega {\varepsilon}_2 {\varepsilon}_o \left\langle E^2 \right\rangle \, ,
$$

which is proportional to the time average of the power of the wave. Its macroscopic form is usually the (Joule) heat.

ntity to be calculated is the energy taken from a harmonic electromagnetic wave in a unit<br>
f time, linked to the imaginary part of the dielectric function,<br>  $Q = \frac{1}{2} \omega \varepsilon_2 \varepsilon_o \langle E^2 \rangle$ ,<br>
bonal to the time average of t The procedure involves a calculation of the increase of the mean energy of the condensed system, and use the above equation for the evaluation of the absorptive part of the dielectric function. The real part can be obtained via Kramers-Kronig transform of the imaginary part calculated for all frequencies.

Matter will be divided into small areas (of the volume *V*, with their dimensions much smaller than the wavelength of the optical field). In these areas, the electric field intensity of the wave is independent of the position; we retain solely the harmonic time dependence *i* to be calculated is the energy tame, linked to the imaginary part  $\epsilon = \frac{1}{2} \omega \varepsilon_2 \varepsilon_o \langle E^2 \rangle$ ,<br> *i* to the time average of the powe ves a calculation of the increase cor the evaluation of the absorptives-Kronig t venient quantity to be calculated is the energy taken from a harmonic electromagn<br>
ne per unit of time, linked to the imaginary part of the dielectric function,<br>  $Q = \frac{1}{2} \cos_2 \mathcal{E}_o \left\langle E^2 \right\rangle$ ,<br>
is proportional to the  $\vec{v}$  calculated is the energy taken from a laked to the imaginary part of the dielect<br>  $\vec{v} \varepsilon_2 \varepsilon_o \langle E^2 \rangle$ ,<br>
e time average of the power of the wave<br>
calculation of the increase of the mean e<br>
evaluation of the a to be calculated is the energy taken from a harmonic electromagnetic wave i<br> *n*, linked to the imaginary part of the dielectric function,<br>  $\frac{1}{2}\omega \varepsilon_2 \varepsilon_o \left\langle E^2 \right\rangle$ ,<br>  $\frac{1}{2}\omega \varepsilon_2 \varepsilon_o \left\langle E^2 \right\rangle$ ,<br>  $\frac{1}{2}\omega \v$ ted is the energy taken from a harm<br>he imaginary part of the dielectric<br> $E^2$ ,  $\left\{ \frac{1}{2} \right\}$ ,<br> $\left\{ \frac{1}{2} \right\}$ ,<br> $\left\{ \frac{1}{2} \right\}$ ,<br> $\left\{ \frac{1}{2} \right\}$ ,<br> $\left\{ \frac{1}{2} \right\}$ ,  $\left\{ \frac{1}{2} \right\}$ ,  $\left\{ \frac{1}{2} \right\}$  and the me convenient quantity to be calculated is the energy taken from a harmonic electromagnetic wave in a unit<br>
ulume per unit of time, linked to the imaginary part of the dielectric function,<br>  $Q = \frac{1}{2} \omega \varepsilon_z \varepsilon_o \left\langle E^2 \right\rangle$ are particular quantity to be calculated is the energy taken from a harmonic electromagnetic wave in a unit<br>me per unit of time, finked to the imaginary part of the dielectric function,<br> $Q = \frac{1}{2} \omega \varepsilon_2 \varepsilon_o \langle E^2 \rangle$ ,<br>h

$$
\vec{E}\left(t\right)=\vec{E}_{o}e^{-i\omega t}
$$

from the time  $t<sub>o</sub>=0$  of switching the perturbation on. Magnetic component will be neglected.

The perturbative part of hamiltonian can be expressed via the operator of dipole moment (charge times its displacement) as

$$
H'(t) = \vec{d} \cdot \text{Re}\left\{\vec{E}_o e^{-i\omega t}\right\} = \frac{\left(\vec{d} \cdot \vec{n}\right)E_o}{2}\left(e^{-i\omega t} + e^{i\omega t}\right), \text{ where } \vec{n} = \vec{E}_o / E_o
$$

is a unit vector in the direction of force. The force performs work due to the displacement of the charge, equal to the scalar product of the vectors of force and displacement.

Assume the system in a stationary state  $i$  (with the energy  $E_i$ ) at the initial time  $t_o$ . The probability of a transition to a stationary final state  $f$  (with the energy  $E_f$ ) at the time  $T$  (which is the squared modolus of the probability amplitude) is

sume the system in a stationary state *i* (with the energy 
$$
E_i
$$
) at the initial time  $t_o$ . The probability of a  
isition to a stationary final state *f* (with the energy  $E_f$ ) at the time *T* (which is the squared modulus of  
probability amplitude) is  

$$
p_{ij}(T, \omega) = \frac{1}{\hbar^2} \left| \left\langle f \left| \int_0^T H'(t) e^{i\frac{E_f - E_i}{\hbar}} dt \right| t \right\rangle \right|^2
$$

$$
= T \left| \left\langle \frac{f}{d} \cdot \vec{n} \right| i \right\rangle \right|^2 \left[ F(T, \omega_{if} - \omega) + F(T, \omega_{if} + \omega) \right] E_o^2, \text{ where}
$$

$$
\omega_{if} = \frac{E_f - E_i}{\hbar}, \quad F(T, x) = \frac{\sin^2 \left( \frac{T}{2} x \right)}{\frac{T}{2} x^2}.
$$
  
therefore  $\omega_{if} = \frac{F_f - E_i}{\hbar}$ , where  $\omega_{if} = \frac{T}{2} x^2$ .  
Therefore, the probability is negligible except for the fullillment of the "resonance condition" $\omega = \pm \omega_{if}$ .

For large *T*, the probability is negligible except for the fulfillment of the "resonance condition"

$$
\omega = \pm \omega_{if}
$$

For  $T \to \infty$  the function *F* can be replaced by the Dirac  $\delta$ :

$$
\int_{-\infty}^{\infty} F(T, x) dx = \pi \text{ for any } T > 0; \quad \lim_{T \to \infty} F(T, x) = \pi \delta(x).
$$

Owing to the transition *i→f* , the light field performs work, which (per unit volume and time) reads

$$
\rightarrow \infty \text{ the function } F \text{ can be replaced by the Dirac } \delta:
$$
\n
$$
\int_{-\infty}^{\infty} F(T, x) dx = \pi \text{ for any } T > 0; \quad \lim_{T \to \infty} F(T, x) = \pi \delta(x).
$$
\n
$$
\text{to the transition } i \rightarrow f, \text{ the light field performs work, which (per unit volume and time) reads}
$$
\n
$$
Q_{if}(\omega) = \frac{\hbar \omega p_{if}(T, \omega)}{TV} \rightarrow \frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2 E_o^2 \left[ \delta(\omega_{if} - \omega) + \delta(\omega_{if} + \omega) \right].
$$

 $\int_{-\infty}^{\infty} F(T, x) dx = \pi$  for any  $T > 0$ ;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br>
the transition  $i \to f$ , the light field performs work, which (per unit<br>  $(\omega) = \frac{\hbar \omega p_{ij}(T, \omega)}{TV} \rightarrow \frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2 E_o^2 \left[ \delta(\omega$ *F*(*T*, *x*)dx =  $\pi$  for any *T* > 0;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br> *F*(*T*, *x*)dx =  $\pi$  for any *T* > 0;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br> **E** transition  $i \to f$ , the light field performs work, which (per unit volume and time)  $\infty$  the function F can be replaced by the Dirac  $\delta$ :<br>  $\int_{-\infty}^{\infty} F(T, x) dx = \pi$  for any  $T > 0$ ;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br>
the transition  $i \to f$ , the light field performs work, which (per unit volume and time) reads<br>  $(\omega$ can be replaced by the Dirac  $\delta$ :<br>
for any  $T > 0$ ;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br>  $\rightarrow f$ , the light field performs work, which (per unity<br>  $\frac{(T, \omega)}{V} \rightarrow \frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2 E_o^2 \left[ \delta(\omega_{if} - \omega) \right]$ <br>
ev c the function F can be replaced by the Dirac  $\delta$ :<br>  $\int_{-\infty}^{\infty} F(T, x) dx = \pi$  for any  $T > 0$ ;  $\lim_{\epsilon \to \infty} F(T, x) = \pi \delta(x)$ .<br>
the transition  $i \to f$ , the light field performs work, which (per unit volume and time) reads<br>  $(\omega) = \$ *i*  $\omega$  the function *F* can be replaced by the Dirac  $\delta$ :<br>  $\int_{-\infty}^{\infty} F(T, x) dx = \pi$  for any  $T > 0$ ;  $\lim_{t \to \infty} F(T, x) = \pi \delta(x)$ .<br>  $\phi$  to the transition  $i \to f$ , the light field performs work, which (per unit volume and tim  $\rightarrow \infty$  the function *F* can be replaced by the Dirac  $\delta$ :<br>  $\int_{-\pi}^{\pi} F(T, x) dx = \pi$  for any  $T > 0$ ;  $\lim_{r \to \infty} F(T, x) = \pi \delta(x)$ .<br> *p* to the transition  $i \rightarrow f$ , the light field performs work, which (per unit volume an<br>  $Q_{if}(\omega$ *F* can be replaced by the Dirac  $\delta$ :<br> *T* for any *T* > 0;  $\lim_{T\to\infty} F(T, x) = \pi\delta(x)$ .<br> *i*  $\rightarrow$  *f*, the light field performs work, which (<br> *i*  $\frac{\partial y}{\partial V}(T, \omega) \rightarrow \frac{\pi\omega}{\hbar V} \left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2 E_o^2 \left[ \delta(T)$ the function  $F$  can be replaced by the Dirac 8:<br>  $\int_{\Gamma} F(T, x) dx = \pi$  for any  $T > 0$ ;  $\lim_{t \to \infty} F(T, x) = \pi \delta(x)$ .<br>
Let transition  $i \to f$ , the light field performs work, which (per unit volume and time) reads<br>  $\omega$ ) =  $\frac{\hbar \omega$ The work vanishes whenever the resonance condition is not fulfilled, and diverges otherwise. This is a consequence of the stationary initial and final states. Quasistationary states have finite lifetimes; for the exponential temporal dependence of the probability *P<sup>s</sup>* of the decay of the state of mean energy *E<sup>o</sup>* during the time  $t(P_n)$  means the probability preserving the state during the time  $t$ ), F can be replaced by the Dirac  $\delta$ :<br>  $\tau$  for any  $T > 0$ ;  $\lim_{T \to \infty} F(T, x) = \pi \delta$ <br>  $\to f$ , the light field performs work, v<br>  $\frac{F(T, \omega)}{\sqrt{V}} \to \frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2 E$ <br>
ever the resonance condition i function F can be replaced by the Dirac  $\delta$ :<br>  $T, x$ )d $x = \pi$  for any  $T > 0$ ;  $\lim_{t \to \infty} F(T, x) = \pi \delta(x)$ .<br>
ansition  $i \to f$ , the light field performs work, which<br>  $= \frac{\hbar \omega p_{if}(T, \omega)}{TV} \rightarrow \frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \$ can be replaced by the Dirac  $\delta$ :<br>
for any  $T > 0$ ;  $\lim_{T \to \infty} F(T, x) =$ <br>  $f$ , the light field performs wor<br>  $\frac{T}{r}$ ,  $\omega$ )  $\Rightarrow \frac{\pi \omega}{\hbar V} \left| \left\langle f | \vec{d} \cdot \vec{n} | i \right\rangle \right|$ <br>  $\int$ <br>  $\int$  rer the resonance condition is r<br>  $\int$  r *P* the function *F* can be replaced by the Dirac  $\delta$ :<br> *F*(*T*, *x*) dx =  $\pi$  for any  $T > 0$ ;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br> *P* transition  $i \to f$ , the light field performs work, which<br> *P*) =  $\frac{\hbar \omega p_{if}(T, \omega)}{TV} \to \frac{\pi \omega}{$ can be replaced by the Dirac  $\delta$ :<br>
for any  $T > 0$ ;  $\lim_{j \to \infty} F(T, x) = \pi \delta(x)$ .<br>  $\rightarrow f$ , the light field performs work, which (per unit volume and time) reads<br>  $\frac{(T, \omega)}{V} \rightarrow \frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2 E_o^2$ tion F can be replaced by the Dirac  $\delta$ :<br>  $dx = \pi$  for any  $T > 0$ :  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br>
tion  $i \to f$ , the light field performs work, which (per unit volume and time) reads<br>  $\frac{\omega p_{\theta}(T, \omega)}{TV} \to \frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \$ by the Dirac  $\delta$ :<br>  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ <br>
performs work, wh<br>  $\left\langle f | \vec{d} \cdot \vec{n} | i \right\rangle|^2 E_o^2$ <br>
condition is not fu<br>
aal states. Quasistat<br>
bability  $P_s$  of the d<br>
ing the state during<br>  $-e^{-\frac{2\Gamma}{\hbar}t}$ ,<br>
is<br>  $\frac{2}{\Gamma +$ function F can be replaced by the Dirac  $\delta$ :<br>  $(\tau, x)dx = \pi$  for any  $T > 0$ ;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ <br>
ansition  $i \to f$ , the light field performs work, which<br>  $= \frac{\hbar \omega p_{ij}(T, \omega)}{TV} \rightarrow \frac{\pi \omega}{\hbar V} \left| \left\langle f | \vec{d} \cdot \vec{n} \right| i \right\rangle \right$ anction *F* can be replaced by the<br> *x*)d*x* = *π* for any *T* > 0;  $\lim_{T\to\infty}$  *F*<br> **E** assistion *i*→*f*, the light field perform<br>  $\frac{\hbar \omega p_{if}(T, \omega)}{TV}$  →  $\frac{\pi \omega}{\hbar V}$   $\left| \left\langle f \left| \frac{\partial T}{\partial T} \right\rangle \right\rangle$ <br>
es whenever t replaced by the Dirac  $\delta$ :<br>  $T > 0$ ;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br>
ight field performs work, which<br>  $\rightarrow \frac{\pi \omega}{\hbar V} \left| \left\langle f | \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2 E_o^2 \left[ \delta \left( \frac{\pi}{\hbar V} \right) \right]$ <br>
resonance condition is not fulfills<br>
ial and f tion F can be replaced by the Dirac  $\delta$ :<br>  $dx = \pi$  for any  $T > 0$ ;  $\lim_{T \to \pi} F(T, x) = \pi \delta(x)$ .<br>
tion  $i \to f$ , the light field performs work, which (per unit volume and time) reads<br>  $\frac{\omega p_{if}(T, \omega)}{TV} \to \frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \vec{$ blaced by the Dirac  $\delta$ :<br>  $>0$ ;  $\lim_{T \to \infty} F(T, x) = \pi \delta(x)$ .<br>
the field performs work, which (per unit volume and time) reads<br>  $\frac{\pi \omega}{\hbar V} \left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2 E_{\sigma}^2 \left[ \delta(\omega_{tf} - \omega) + \delta(\omega_{tf} + \omega) \right]$ .<br>
conance c

$$
P_n(t) = e^{-\frac{2\Gamma}{\hbar}t} , \quad P_s(t) = 1 - e^{-\frac{2\Gamma}{\hbar}t} ,
$$

the probability density of finding energy *E* is

$$
\rho(E - Eo) = \frac{\Gamma}{\pi} \frac{1}{(E - Eo)^2 + \Gamma^2} .
$$

This is so called Breit-Wigner, or Lorentz, or Cauchy distribution.

The positive parameter  $\Gamma$  has the dimension of energy; it is inversely proportional to the lifetime of quasistationary  $(\Gamma \ll E_o)$  state,

$$
\tau = \frac{h}{2\Gamma} \; .
$$

For  $\Gamma \to 0$   $(\tau \to \infty)$ ,  $\rho(E-E_{\rho}) \to \delta(E-E_{\rho})$ .

Thus, the Fermi golden rule of the perturbation theory can be complemented by the assumption concerning the random values of the energy

$$
E_{if}=E_{f}-E_{i}=\hbar\omega_{if}
$$

nension of energy; it is inversely proportional to the lifetime of<br>  $=\frac{\hbar}{2\Gamma}$ .<br>  $-E_o$ )  $\rightarrow \delta(E - E_o)$ .<br>
rturbation theory can be complemented by the assumption concerning<br>  $= E_f - E_i = \hbar \omega_{if}$ <br>
sition. The width parameters of taken from the wave via the *i→f* transition. The width parameters of the Breit-Wigner distribution of the initial and final energies can differ; assuming independent occurrence of both energies, the probability density of the energy difference is the convolution (Faltung, svjortka)

2 2 2 2 2 2 / / ( ) d ( ) ( ) ( ) / . ( ) ( ) *f i if o o f f f i i i i f o if if i f E E E E E E E E E E* 0 ( ) , ( ) ( ) . *E E E E o o E E E if f i if*

This is again the Breit-Wigner distribution; it is centered about the difference of the individual centers.

The width parameters and the corresponding relaxation times are

h parameters and the corresponding relaxation times are  
\n
$$
\Gamma_{if} = \Gamma_i + \Gamma_f, \qquad \frac{1}{\tau_{if}} = \frac{\hbar}{2\Gamma_{if}} = \frac{1}{\tau_i} + \frac{1}{\tau_f}.
$$
\ninterpretation of inverse relaxation time as the frequency of  
\noncerning the initial and final states is the sum of frequencies  
\ntral dependence of the energy absorbed via transitions *i*→*f*  
\nred version of the delta-function singularity for stationary sta  
\nand summation over all possibilities leads to

With the interpretation of inverse relaxation time as the frequency of collisions, the result for independent events concerning the initial and final states is the sum of frequencies.

The spectral dependence of the energy absorbed via transitions *i→f* between quasistationary states is broadened version of the delta-function singularity for stationary states. Multiplication by the probability density and summation over all possibilities leads to corresponding relaxation times are<br>  $\frac{1}{\tau_{if}} = \frac{\hbar}{2\Gamma_{if}} = \frac{1}{\tau_i} + \frac{1}{\tau_f}$ .<br> *is insert in the interpret in the frequency of collisions, the result for independent*<br> *ind final states is the sum of frequencies.*<br> h parameters and the corresponding relaxation times are<br>  $\Gamma_{if} = \Gamma_i + \Gamma_f$ ,  $\frac{1}{\tau_{if}} = \frac{\hbar}{2\Gamma_{if}} = \frac{1}{\tau_i} + \frac{1}{\tau_f}$ .<br>
interpretation of inverse relaxation time as the frequency of collisions, the result for independen  $\omega = \pm \omega_{if}$ .<br>  $\omega = \pm \omega_{if}$ .

th parameters and the corresponding relaxation times are  
\n
$$
\Gamma_{ij} = \Gamma_i + \Gamma_j, \quad \frac{1}{\tau_{ij}} = \frac{\hbar}{2\Gamma_{ij}} = \frac{1}{\tau_i} + \frac{1}{\tau_j}.
$$
\ninterpretation of inverse relaxation time as the frequency of collisions, the result for independent  
\noneering the initial and final states is the sum of frequencies.  
\ntrral dependence of the energy absorbed via transitions  $i \rightarrow f$  between quasistationary states is  
\ned version of the delta-function singularity for stationary states. Multiplication by the probability  
\nand summation over all possibilities leads to  
\n
$$
\int_{-\infty}^{\infty} \left[ \delta(\omega_{if} - \omega) + \delta(\omega_{if} + \omega) \right] \rho(\hbar \omega_{if}) d(\hbar \omega_{if})
$$
\n
$$
= \int_{-\infty}^{\infty} \left[ \delta(x/\hbar - \omega) + \delta(x/\hbar + \omega) \right] \rho(x) d(x)
$$
\n
$$
= \hbar \rho(\hbar \omega) + \hbar \rho(-\hbar \omega)
$$
\n
$$
= \hbar \frac{\Gamma_{ij}}{\pi} \left[ \frac{1}{(\hbar \omega - \hbar \omega_{ij}^o)^2 + \Gamma_{ij}^2} + \frac{1}{(\hbar \omega + \hbar \omega_{ij}^o)^2 + \Gamma_{ij}^2} \right].
$$
\n\nnameses are of finite magnitude and width, they are centered close to  
\n
$$
\omega = \pm \omega_{ij}
$$

The resonances are of finite magnitude and width, they are centered close to

$$
\omega = \pm \omega_{if} .
$$

The former result leads to the following approximate expression for the contribution of the *i→f* transitions to the imaginary part of the dielectric function,

For a result leads to the following approximate expression for the contribution of the *i*→*f* transitions

\nequary part of the dielectric function,

\n
$$
(\Delta \varepsilon_2)_{if} = \frac{2Q_{if}}{\omega \varepsilon_o \left\langle E^2 \right\rangle} = \frac{4Q_{if}}{\omega \varepsilon_o E_o^2}
$$
\n
$$
\approx \frac{4}{\varepsilon_o} \frac{\left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2}{V} \left[ \frac{\Gamma_{if}}{\left( \hbar \omega - \hbar \omega_{if}^o \right)^2 + \Gamma_{if}^2} - \frac{\Gamma_{if}}{\left( \hbar \omega + \hbar \omega_{if}^o \right)^2 + \Gamma_{if}^2} \right].
$$
\nand can be further simplified, and, the need for the Kramers-Kronig transform (to obtain the real

\nideal.

This formula can be further simplified, and, the need for the Kramers-Kronig transform (to obtain the real part) avoided.

Since

$$
\frac{\gamma}{(\omega - \omega_o)^2 + \gamma^2} - \frac{\gamma}{(\omega + \omega_o)^2 + \gamma^2}
$$
\n
$$
= \text{Im}\left\{\frac{1}{\omega_o - \omega - i\gamma} + \frac{1}{\omega_o + \omega + i\gamma}\right\} = \text{Im}\left\{\frac{2\omega_o}{\omega_o^2 + \gamma^2 - \omega^2 - i2\omega\gamma}\right\},
$$
\npartition to the absorptive part of the dielectric function can be expressed in the form

\n
$$
(\Delta \varepsilon_2)_{if} = \frac{4}{\varepsilon_o} \frac{\left|\left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle\right|^2}{V} \frac{2\omega_{if}^o}{\hbar} \text{Im}\left\{\frac{1}{(\omega_{if}^o)^2 + \frac{\Gamma_{if}^2}{\hbar^2} - \omega^2 - i\omega\frac{2\Gamma_{if}}{\hbar}\right\}}\right\}.
$$
\nis to be compared with the result of classical Lorentz model for the complex dielectric function,

\n
$$
\varepsilon = 1 + \frac{S\omega_o^2}{\omega_o^2 - \omega^2 - i\frac{\omega}{\tau}}.
$$

the contribution to the absorptive part of the dielectric function can be expressed in the form

$$
= \text{Im}\left\{\frac{1}{\omega_o - \omega - i\gamma} + \frac{1}{\omega_o + \omega + i\gamma}\right\} = \text{Im}\left\{\frac{2\omega_o}{\omega_o^2 + \gamma^2 - \omega^2 - i2\omega\gamma}\right\}
$$
\npartition to the absorptive part of the dielectric function can be expressed in the

\n
$$
(\Delta \varepsilon_2)_{if} = \frac{4}{\varepsilon_o} \frac{\left|\left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle\right|^2}{V} \frac{2\omega_{if}^{\circ}}{\hbar} \text{Im}\left\{\frac{1}{(\omega_{if}^{\circ})^2 + \frac{\Gamma_{if}^2}{\hbar^2} - \omega^2 - i\omega\frac{2\Gamma_{if}}{\hbar}\right\}}{(\omega_{if}^{\circ})^2 + \frac{\Gamma_{if}^2}{\hbar^2} - \omega^2 - i\omega\frac{2\Gamma_{if}}{\hbar}\right\}}
$$
\nso be compared with the result of classical Lorentz model for the complex dielole

\n
$$
\varepsilon = 1 + \frac{S\omega_o^2}{\omega_o^2 - \omega^2 - i\frac{\omega}{\tau}}.
$$

This is to be compared with the result of classical Lorentz model for the complex dielectric function,

$$
\varepsilon = 1 + \frac{S\omega_o^2}{\omega_o^2 - \omega^2 - i\frac{\omega}{\tau}}.
$$

The dimensionless "strength" of the *i→f* transitions is

nless "strength" of the *i*→*f* transitions is  
\n
$$
S_{if} = \frac{8}{\varepsilon_o \hbar \omega_{if}^o} \frac{|\langle f | \vec{d} \cdot \vec{n} | i \rangle|^2}{V},
$$
\n\nuency and damping time are  
\n
$$
\omega_{o,if} = \sqrt{(\omega_{if}^o)^2 + \frac{\Gamma_{if}^2}{\hbar^2}}, \quad \tau_{if} = \frac{\hbar}{2\Gamma_{if}}.
$$
\nspectral dependencies of the imaginary parts  
\nred by Kramers-Kronig integral transform. The  
\nshort contributions of transitions from differ  
\nspersive (real) part of the dielectric function

the eigenfrequency and damping time are

onless "strength" of the *i*→*f* transitions is  
\n
$$
S_{if} = \frac{8}{\varepsilon_o \hbar \omega_{if}^o} \frac{|\langle f | \vec{d} \cdot \vec{n} | i \rangle|^2}{V},
$$
\n\nquency and damping time are  
\n
$$
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$$
\n1 spectral dependencies of the imaginary parts imply identical so

ess "strength" of the  $i \rightarrow f$  transitions is<br>  $\int_{if}$  =  $\frac{8}{\varepsilon_o \hbar \omega_{if}^o} \frac{|\langle f | \vec{d} \cdot \vec{n} | i \rangle|^2}{V}$ ,<br>
mey and damping time are<br>  $\int_{if} = \sqrt{(\omega_{if}^o)^2 + \frac{\Gamma_{if}^2}{\hbar^2}}$ ,  $\tau_{if} = \frac{\hbar}{2\Gamma_{if}}$ .<br>
ectral dependencies of th thess "strength" of the  $i\rightarrow f$  transitions<br>  $S_{if} = \frac{8}{\varepsilon_o \hbar \omega_{if}^o} \frac{\left| \left\langle f | \vec{d} \cdot \vec{n} | i \right\rangle \right|^2}{V}$ ,<br>
ency and damping time are<br>  $\omega_{o,if} = \sqrt{(\omega_{if}^o)^2 + \frac{\Gamma_{if}^2}{\hbar^2}}$ ,  $\tau_{if} = \frac{1}{2I}$ <br>
pectral dependencies of t onless "strength" of the  $i\rightarrow f$  transitions is<br>  $S_{ij} = \frac{8}{\epsilon_o \hbar \omega_{ij}^o} \frac{\left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2}{V}$ ,<br>
wency and damping time are<br>  $\omega_{o,jf} = \sqrt{(\omega_{ij}^o)^2 + \frac{\Gamma_{ij}^2}{\hbar^2}}$ ,  $\tau_{ij} = \frac{\hbar}{2\Gamma_{ij}}$ .<br>
I spectral de "strength" of the  $i \rightarrow f$  transitions is<br>  $= \frac{8}{\varepsilon_o \hbar \omega_g^o} \frac{\left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2}{V}$ ,<br>
and damping time are<br>  $= \sqrt{(\omega_g^o)^2 + \frac{\Gamma_f^2}{\hbar^2}}$ ,  $\tau_{ij} = \frac{\hbar}{2\Gamma_{ij}}$ .<br>
and dependencies of the imaginary parts i "strength" of the  $i \rightarrow f$  transitions is<br>  $= \frac{8}{\varepsilon_o \hbar \omega_{if}^o} \frac{\left| \left\langle f | \vec{d} \cdot \vec{n} | i \right\rangle \right|^2}{V}$ ,<br>
and damping time are<br>  $= \sqrt{(\omega_{if}^o)^2 + \frac{\Gamma_{if}^2}{\hbar^2}}$ ,  $\tau_{if} = \frac{\hbar}{2\Gamma_{if}}$ .<br>
al dependencies of the imaginary parts s "strength" of the  $i\rightarrow f$  transitions is<br>  $= \frac{8}{\varepsilon_o \hbar \omega_q^o} \frac{\left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2}{V}$ ,<br>
y and damping time are<br>  $= \sqrt{(\omega_q^o)^2 + \frac{\Gamma_q^2}{\hbar^2}}$ ,  $\tau_{q} = \frac{\hbar}{2\Gamma_{q}}$ .<br>
transl dependencies of the imaginary e  $i \rightarrow f$  transitions is<br>  $\left| \frac{\vec{d} \cdot \vec{n} |i}{v} \right|^2$ <br>  $\frac{\vec{a} \cdot \vec{n}}{v^2}$ ,  $\tau_{ij} = \frac{\hbar}{2\Gamma_{ij}}$ .<br>
So for the imaginary parts imply identical spectra of the real parts, since<br>
gintegral transitions from different initial ngth" of the  $i \rightarrow f$  transitions is<br>  $\frac{8}{8} \frac{\left| \left\langle f \right| \vec{d} \cdot \vec{n} \left| i \right\rangle \right|^2}{V}$ ,<br>  $i \omega_{ij}^0$ ,  $V$ <br>  $\left| \frac{\partial \omega_{ij}^0}{\partial t} \right|^2 + \frac{\Gamma_{ij}^2}{\hbar^2}$ ,  $\tau_{ij} = \frac{\hbar}{2\Gamma_{ij}}$ .<br>
pendencies of the imaginary parts imply identical of the  $i \rightarrow f$  transitions is<br>  $\left\langle f | \vec{d} \cdot \vec{n} | i \right\rangle^2$ <br>  $V$ ,<br>  $\frac{1}{2} \sum_{i} \vec{n}$ ,<br>  $\frac{1}{n^2}$ ,  $\tau_{ij} = \frac{\hbar}{2\Gamma_{ij}}$ .<br>
Acies of the imaginary parts imply identical spectra of the real parts, since<br>
conig integral trans The identical spectral dependencies of the imaginary parts imply identical spectra of the real parts, since they are related by Kramers-Kronig integral transform. Thus, in summing the contributions of (possibly many) independent contributions of transitions from different initial states to different final states, we may include the dispersive (real) part of the dielectric function in the sum: trength" of the *i*- $f$  transitions is<br>  $\frac{8}{\varepsilon_o \hbar \omega_v^o} \frac{\left| \left\langle f | \vec{d} \cdot \vec{n} | i \right\rangle \right|^2}{V}$ ,<br>
and damping time are<br>  $\sqrt{(\omega_y^o)^2 + \frac{\Gamma_y^2}{\hbar^2}}$ ,  $\tau_{ij} = \frac{\hbar}{2\Gamma_{ij}}$ .<br>
dependencies of the imaginary parts imply identi

s "strength" of the *i*–*f* transitions is  
\n
$$
= \frac{8}{\varepsilon_o \hbar \omega_{ij}^o} \frac{\left| \left\langle f \left| \vec{d} \cdot \vec{n} \right| i \right\rangle \right|^2}{V},
$$
\ny and damping time are  
\n
$$
= \sqrt{(\omega_{ij}^o)^2 + \frac{\Gamma_{ij}^2}{\hbar^2}}, \quad \tau_{ij} = \frac{\hbar}{2\Gamma_{ij}}.
$$
\nstral dependencies of the imaginary parts imply identical spectra  
\ny Kramers-Kronig integral transform. Thus, in summing the cont  
\nnot contributions of transitions from different initial states to differ  
\nsive (real) part of the dielectric function in the sum:  
\n
$$
\varepsilon(\omega) = 1 + \sum_{i,f} \frac{S_{ij} \omega_{o,ij}^2}{\omega_{o,ij}^2 - \omega^2 - i \frac{\omega}{\tau_{ij}}.
$$
\nhas poles in the lower plane of complex frequencies.

Each of the terms has poles in the lower plane of complex frequencies.

The matrix element involving the charge and position,

$$
D_{ij} = \langle f | \vec{d} \cdot \vec{n} | i \rangle = e \langle f | \vec{r} \cdot \vec{n} | i \rangle ,
$$

can be expressed in terms of the momentum operator, using the commutator of the unperturbed hamiltonian *H<sup>o</sup>* with the position:

ix element involving the charge and position,  
\n
$$
D_{if} = \langle f | \vec{d} \cdot \vec{n} | i \rangle = e \langle f | \vec{r} \cdot \vec{n} | i \rangle,
$$
\n
$$
p_{\text{pressed in terms of the momentum operator, using the commutator of the unperturbed}
$$
\n
$$
\langle f | H_o \vec{r} | i \rangle = E_f \langle f | \vec{r} | i \rangle , \langle f | \vec{r} H_o | i \rangle = E_i \langle f | \vec{r} | i \rangle ,
$$
\n
$$
\langle f | [H_o, \vec{r}] | i \rangle = (E_f - E_i) \langle f | \vec{r} | i \rangle ,
$$
\n
$$
\langle f | \vec{r} | i \rangle = \frac{\langle f | [H_o, \vec{r}] | i \rangle}{E_f - E_i}.
$$
\n
$$
[H_o, \vec{r}] = -i\hbar \frac{d\vec{r}}{dt} = -i\hbar \frac{\vec{P}}{m},
$$
\nat\n
$$
D_{if} = -i \frac{e\hbar}{m(E_f - E_i)} \langle f | \vec{p} \cdot \vec{n} | i \rangle .
$$
\n39

Since

$$
[H_o, \vec{r}] = -i\hbar \frac{d\vec{r}}{dt} = -i\hbar \frac{\vec{p}}{m}
$$

we arrive at

$$
D_{if} = -i \frac{e\hbar}{m(E_f - E_i)} \langle f | \vec{p} \cdot \vec{n} | i \rangle .
$$

The transition probability is proportional to

$$
\left| D_{ij} \right|^2 = \left| \frac{e\hbar}{m(E_{f}-E_{i})} \right|^2 \left| \left\langle f \left| \vec{p} \cdot \vec{n} \right| i \right\rangle \right|^2 \; .
$$

This form is usually used for the one-electron transitions in crystals, which do not involve other excitations (such as phonons). As the momentum is proportional to the *k*–vector of the Bloch states, the matrix element is zero for states of different *k* (the state vectors are orthogonal). The allowed transitions are called "direct" (in *k*-space). This selection rule can also be interpreted as the requirement of momentum conservation, since the momentum of the involved photon is negligible. brobability is proportional to<br>  $\left| \int_{if}^{2} e^{-\frac{1}{2}} \frac{e^{\frac{1}{2}}}{m(E_f - E_i)} \right|^2 \left| \left\langle f | \vec{p} \cdot \vec{n} \right| i \right|^2$ .<br>  $\left| \int_{if}^{2} e^{-\frac{1}{2}} \frac{1}{m(E_f - E_i)} \right|^2 \left| \int_{if}^{2} \vec{p} \cdot \vec{n} \right| i^2$ .<br>  $\left| \int_{if}^{2} \vec{n} \right| \leq \frac{1}{2}$ <br>  $\left| \int_{if}^{2$ proportional t<br>  $\left.\frac{e\hbar}{f-E_i}\right|^2$   $\left|\left\langle j\right|\right|$ <br>
the one-elect<br>
infferent *k* (the<br>
lection rule cantum of the i *eh*  $D_{if} \Big|^{2} = \left| \frac{e\hbar}{m(E_{f} - E_{i})} \right|^{2} \Big| \Big\langle f | \vec{p} \cdot \vec{n} | i \rangle \Big|^{2}$ .<br> *ehere*  $M_{if} \Big| \Big| \Big\langle E_{if} - E_{if} \Big| \Big| \Big| \Big\langle f | \vec{p} \cdot \vec{n} | i \rangle \Big|^{2}$ *.*<br> *ending ii* and the one-electron transitions in cry and the *k*-v or o ability is proportional to<br>  $=\left|\frac{e\hbar}{m(E_f - E_i)}\right|^2 \left|\left\langle f|\vec{p} \cdot \vec{n}|i\rangle\right|^2\right|$ .<br>  $\therefore$ <br>  $\therefore$  used for the one-electron transitions in crystals, which do not involve other excitations<br>
As the momentum is proportional to