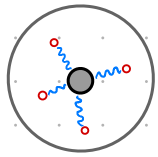
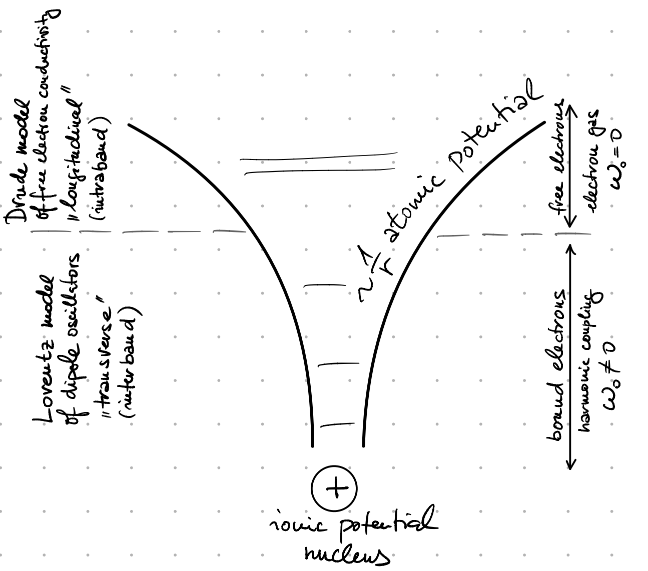
3) Classical light propagation



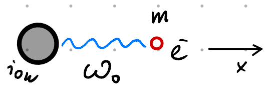
electrons are held to heavy nucleus by springs, which represent the restoring forces

- light is treated as electromagnetic waves and atoms are modelled as classical oscillators

Electrons respond to an external field $\vec{E}(t)$ by accelerating + damping due to collisions called Drude-Lorentz model (application of oscillator model to free $\bar{e}$ systems)



$$m\ddot{x} + m\gamma\dot{x} + m\omega_0^2 x = -eE(t)$$



$$E(t) = E_0 e^{-i\omega t}$$

ac field

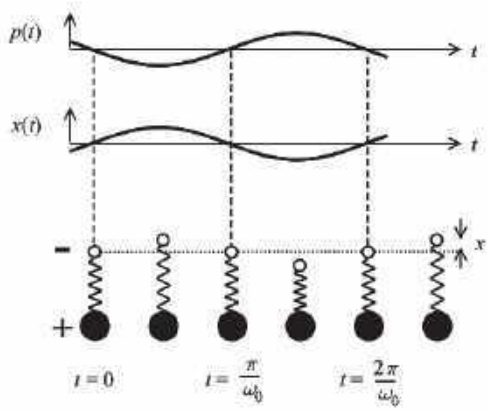
γ is the damping rate of the oscillator

Solution is seek as $x(t) = X_0 e^{-i\omega t}$ leading to

$$X_0 = \frac{eE_0/m}{\omega^2 - \omega_0^2 + i\gamma\omega}$$

displacement of electrone $x(t)$ from their equilibrium positions produces time varying dipole moment

$$p(t) = -ex(t)$$



Giving contribution to macroscopic resonant polarization

$$P = np = -nex = -\frac{e^2 n}{m}\frac{E_0}{\omega^2 - \omega_0^2 + i\gamma\omega}$$

numbers of atoms per unit volume

Dielectric displacement $\vec{D} = \varepsilon_0\vec{E} + \vec{P}$

as we are interested in the optical response close to ω_0 we can split the polarization into non-resonant background and resonant terms

$$\vec{D} = \varepsilon_0\vec{E} + \vec{P}_{background} + \vec{P} = \varepsilon_0\vec{E} + \varepsilon_0\chi\vec{E} + \vec{P}$$

↳ electric susceptibility of background

We can define the relative dielectric constant $\vec{D} = \varepsilon_0\varepsilon_r\vec{E}$

$$\varepsilon_r(\omega) = 1 + \chi - \frac{e^2 n}{\varepsilon_0 m}\frac{1}{\omega^2 - \omega_0^2 + i\gamma\omega}$$

and split to real and imaginary parts

$$\varepsilon_1(\omega) = 1 + \chi + \frac{e^2 n}{\varepsilon_0 m}\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}$$

$$\varepsilon_2(\omega) = \frac{e^2 n}{\varepsilon_0 m}\frac{\gamma\omega}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}$$

Generalization for many oscillators

$$\varepsilon_r(\omega) = 1 + \chi + \frac{e^2 n}{\varepsilon_0 m}\sum_j \frac{1}{\omega^2 - \omega_j^2 + i\gamma_j\omega}$$

Limit cases

$$\omega \to 0 : \quad \varepsilon_r(0) \equiv \varepsilon_{st} = 1 + \chi + \frac{e^2 N}{\varepsilon_0 m \omega_0^2} \qquad \text{(static)}$$

$$\omega \to \infty : \quad \varepsilon_r(\infty) \equiv \varepsilon_\infty = 1 + \chi$$

$$\varepsilon_{st} - \varepsilon_\infty = \frac{e^2 N}{\varepsilon_0 m \omega_0^2} > 0$$

$$\varepsilon_r = \varepsilon_\infty + (\varepsilon_{st} - \varepsilon_\infty) \frac{\omega_0^2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

by introducing detuning $\Delta\omega = \omega - \omega_0$

$$\varepsilon_1(\Delta\omega) = \varepsilon_\infty - (\varepsilon_{st} - \varepsilon_\infty) \frac{2\omega_0 \Delta\omega}{4(\Delta\omega)^2 + \gamma^2}$$

$$\varepsilon_2(\Delta\omega) = (\varepsilon_{st} - \varepsilon_\infty) \frac{\gamma\omega_0}{4(\Delta\omega)^2 + \gamma^2}$$

describe a sharp absorption centered at ω_0 with full width at half maximum equal to γ (Lorentian)

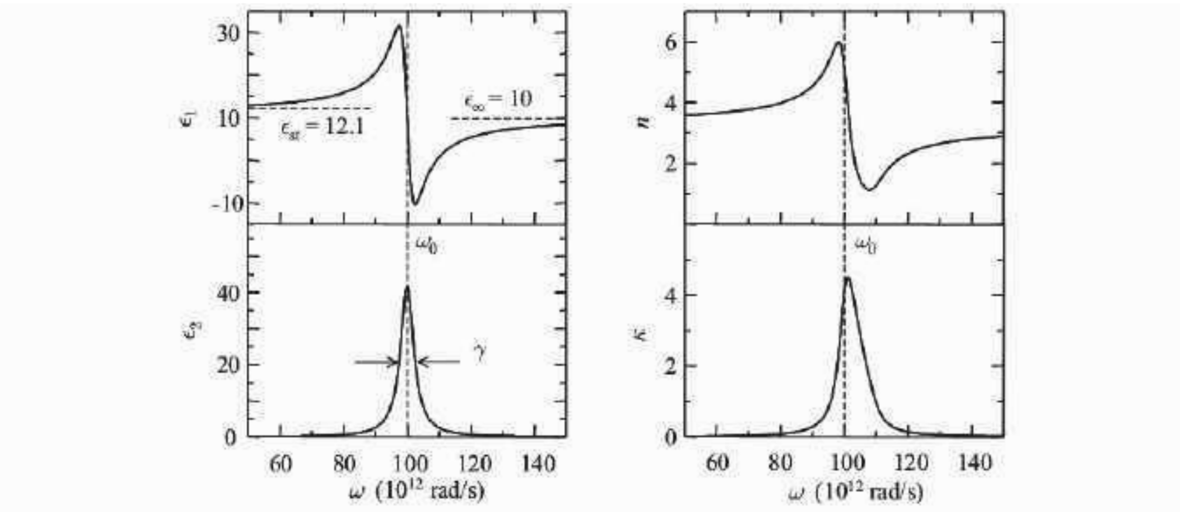


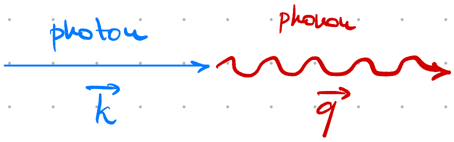
Fig. 2.4 Frequency dependence of the real and imaginary parts of the complex dielectric constant of a dipole oscillator at frequencies close to resonance. The graphs are calculated for an oscillator with $\omega_0 = 10^{14}$ rad/s, $\gamma = 5 \times 10^{12}\ s^{-1}$, $\epsilon_{st} = 12.1,0$ and $\epsilon_\infty = 10$. Also shown is the real and imaginary part of the refractive index calculated from the dielectric constant.

Src: M. Fox book

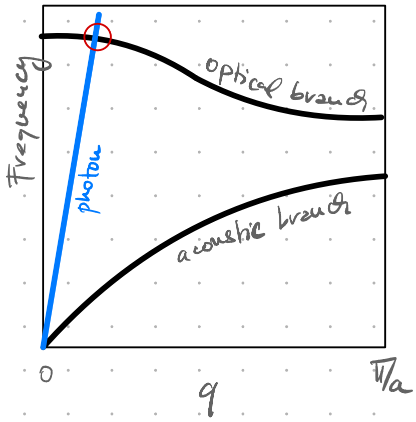
Fox p. 271

EXAMPLE: Infrared activity in polar crystals

resonant frequencies of the phonons that interact with the light are in the infrared spectral region $\longrightarrow$ infrared active modes



Lattice absorption process by an infrared active phonon



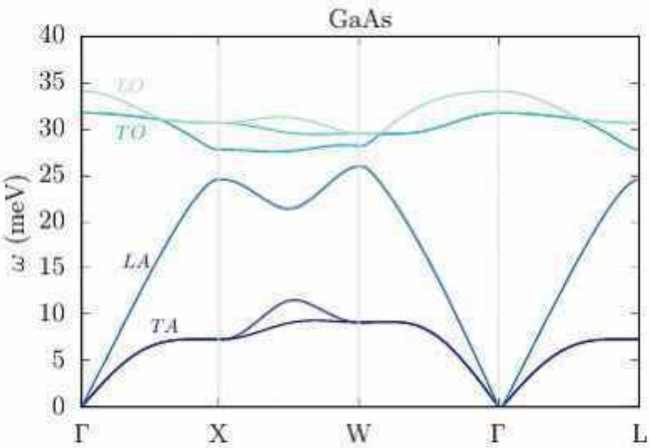
photon dispersion has a constant slope in the crystal $v = c/n$

since $c/n \gg v_s$ $\Rightarrow$ photon dispersion intersects for non zero $\vec{q}$ is for optical phonons, which are flat therefore the resonant frequency is equal to the frequency at $\vec{q} = 0$

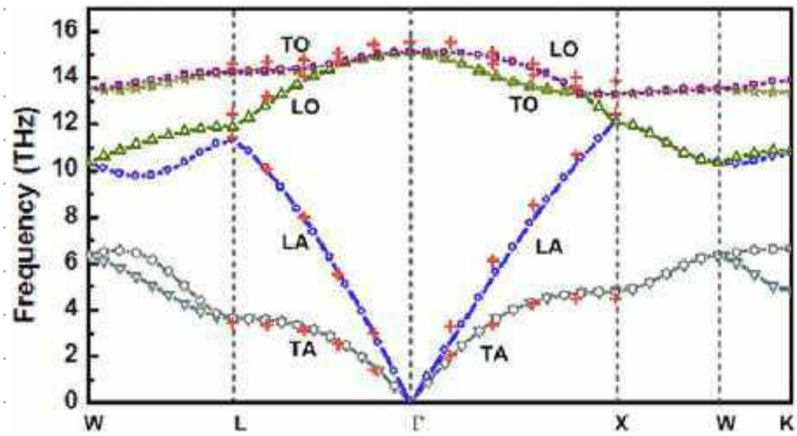
Elmag. waves are transverse thus couple to transverse crystal vibrations, i.e., transverse optical modes only.

Infrared activity of the phonon modes in polar and non-polar crystals. LA: longitudinal acoustic, TA: transverse acoustic, LO: longitudinal optic, TO: transverse optic.

Mode	Polar crystal	Non-polar crystal
LA	no	no
TA	no	no
LO	no	no
TO	yes	no



silicon



4) Optics of free electrons

A) Plasma reflectivity

we set in Drude – Lorentz model $\omega_0 = 0$ (no background)

$$\varepsilon(\omega) = 1 - \frac{ne^2}{\varepsilon_0 m} \frac{1}{(\omega^2 + i\gamma\omega)} = 1 - \frac{\Omega_p^2}{(\omega^2 + i\gamma\omega)} \qquad (1)$$

$$\Omega_p = \left(\frac{ne^2}{\varepsilon_0 m}\right)^{1/2} \quad \text{plasma frequency}$$

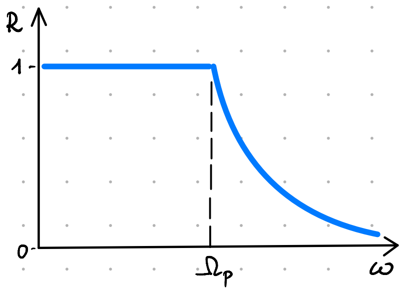
if $\gamma = 0$; $\varepsilon(\omega) = 1 - \frac{\Omega_p^2}{\omega^2}$

Remember : $\tilde{n} = \sqrt{\varepsilon} \implies$ $\tilde{n}$ is imaginary for $\omega < \Omega_p$
$\tilde{n}$ is positive for $\omega > \Omega_p$
$\tilde{n} = 0$ at $\omega = \Omega_p$

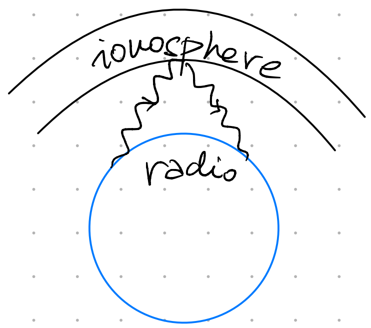
$\tilde{n}^2 = \varepsilon < 0 \Rightarrow \tilde{n} = i\kappa$; $\kappa = \sqrt{|\varepsilon|}$

$$R = \left|\frac{\tilde{n} - 1}{\tilde{n} + 1}\right|^2 = \left|\frac{i\kappa - 1}{i\kappa + 1}\right|^2 = \frac{1 + \kappa^2}{1 + \kappa^2} = 1$$

! negative dielectric constant means perfect reflectivity"



Remember :



atoms are ionized by sun's UV light
plasma frequency $\approx$ MHz

FM waves are transmitted
AM waves are reflected

at night the ionosphere is charged by cosmic rays only, which means less ionization

B) Free carrier conductivity

As we can write the Drude-Lorentz model for $\omega_0 = 0$, i.e., Drude model

$$m \frac{d\vec{v}}{dt} + m\gamma \vec{v} = -e\vec{E}$$

and $m\vec{v} = \vec{p}$ we see that

$$\frac{d\vec{p}}{dt} = -\frac{\vec{p}}{\tau} - e\vec{E}$$

electrons are accelerated by the field but loses its momentum in time τ where $\tau = 1/\gamma$ is the damping time

In AC field $\vec{E}(t) = \vec{E}_0 e^{-i\omega t}$ we find solution in the form

$$\vec{v}(t) = \vec{v}_0 e^{-i\omega t}$$

$$\vec{v}(t) = \frac{-e\tau}{m} \frac{1}{1-i\omega\tau} \vec{E}(t)$$

Note: in Drude model electron gas moves as a uniform see of charge along the field $\vec{E}(t)$

The current density $\vec{j} = -ne\vec{v} = \sigma \vec{E}$

$\sigma \to$ electrical conductivity

From above we get

$$\sigma(\omega) = \frac{\sigma_0}{1-i\omega\tau} \qquad \text{where } \sigma_0 = \frac{ne^2\tau}{m} \text{ is DC conductivity}$$

$\tau = 10^{-14} - 10^{-13}\,s$ for typical metals

Comparing $\sigma(\omega)$ with $\varepsilon(\omega)$ we find mutual relation

$$\boxed{\varepsilon(\omega) = 1 + \frac{i\sigma(\omega)}{\varepsilon_0 \omega}}$$

optical measurements are equivalent to AC conductivity measurements

Indeed hold

$$1 + \frac{i\sigma(\omega)}{\varepsilon_0\omega} = 1 + i\Omega_p^2 \frac{1}{\frac{\omega}{\tau} - i\omega^2} = 1 + \Omega_p^2 \frac{1}{-\frac{i\omega}{\tau} - \omega^2}$$

$$= 1 - \frac{\Omega_p^2}{\omega^2 + i\frac{\omega}{\tau}}$$

$$\varepsilon_1(\omega) = 1 - \frac{\Omega_p^2 \tau^2}{1+\omega^2\tau^2}$$

$$\varepsilon_2(\omega) = \frac{\Omega_p^2 \tau}{\omega} \frac{1}{1+\omega^2\tau^2}$$

EXAMPLE: Skin effect

- Optical conductivity of a free electron gas in the Drude model is

$$\sigma(\omega) = \frac{ne^2}{m}\frac{\tau}{1-i\omega\tau} = \varepsilon_0 \Omega_p^2 \frac{\tau}{1-i\omega\tau}$$

we know that

$$\varepsilon(\omega) = 1 - \frac{\Omega_p^2}{\omega^2 + i\gamma\omega} = 1 + \frac{i\sigma(\omega)}{\varepsilon_0\omega}$$

check: $$1 + \frac{i\sigma(\omega)}{\varepsilon_0\omega} = 1 + i\Omega_p^2 \frac{1}{\frac{\omega}{\tau} - i\omega^2} = 1 + \Omega_p^2 \frac{1}{-\frac{i\omega}{\tau} - \omega^2} =$$

$$= 1 - \frac{\Omega_p^2}{\omega^2 + i\frac{\omega}{\tau}} \quad ; \quad \gamma \equiv \frac{1}{\tau} \text{ ... broadening}$$

thus: $$\varepsilon_1(\omega) = 1 - \frac{\Omega_p^2\tau^2}{1+\omega^2\tau^2}$$

$$\varepsilon_2(\omega) = \frac{\Omega_p^2}{\omega}\frac{\tau}{1+\omega^2\tau^2}$$

typical relaxation time $\tau \approx 10^{-14} - 10^{-13}\,s$

Let $\omega\tau \ll 1$, low frequencies case

$$\varepsilon_2(\omega) = \frac{(\Omega_p\tau)^2}{\omega\tau} \gg \varepsilon_1 \approx 1 - (\Omega_p\tau)^2$$

$$\kappa \approx \sqrt{\varepsilon_2/2}$$

$$n \approx \sqrt{\varepsilon_2/2} \approx \kappa$$

$$\alpha = \frac{2\kappa\omega}{c} = \frac{2\omega}{c}\sqrt{\frac{\varepsilon_2}{2}} = \frac{\omega}{c}\sqrt{2\frac{\Omega_p^2\tau}{\omega}} = \sqrt{\frac{2\Omega_p^2(\tau\omega)}{c^2}} =$$

$$= \left| \begin{array}{l} \Omega_p^2\tau = \sigma(0)/\varepsilon_0 \\ c^2 = \frac{1}{\varepsilon_0\mu_0} \end{array} \right| = \sqrt{2\sigma(0)\omega\mu_0}$$

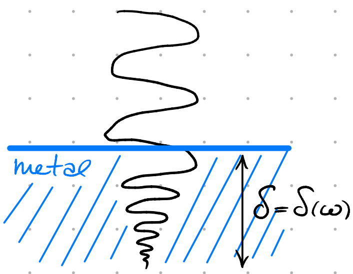
↳ DC conductivity $\equiv \sigma_0$

$$I(z) = I_0 e^{-\alpha z}$$

$$E = E_0 e^{-\alpha z/2} = E_0 e^{-z/\delta}$$

$$\boxed{\delta = \frac{2}{\alpha} = \left(\frac{2}{\sigma_0\omega\mu_0}\right)^{1/2}}$$

Skin depth



5) Comparison of bound and free electron models

$$\varepsilon_1(\omega) = 1 + \chi + \frac{\Omega_p^2(\omega_0^2-\omega^2)}{(\omega^2-\omega_0^2) + (\gamma\omega)^2}$$

$$\varepsilon_2(\omega) = \frac{\Omega_p^2}{(\omega^2-\omega_0^2)+(\gamma\omega)^2}$$

$$\Omega_p = \left(\frac{ne^2}{\varepsilon_0 m}\right)^{1/2}$$

$$\Omega_p \approx 0.716\left(\frac{1}{r_s/a_0}\right)^{3/2} \times 10^{17}\ Hz$$

Free electron model :
$\omega_0 = 0$ & $\chi = 0$

$a_0 = 0.512\,Å$ Bohr radius

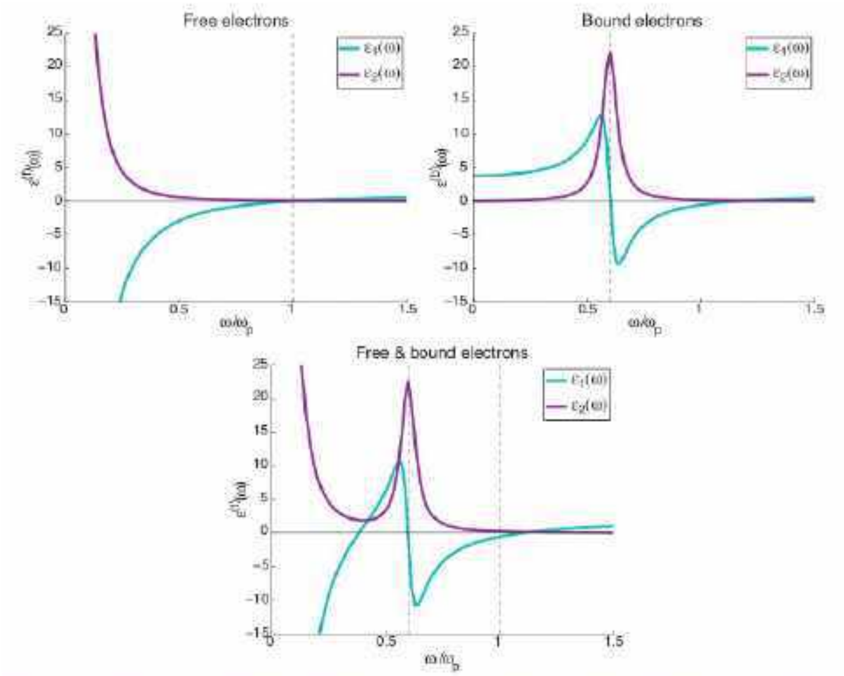
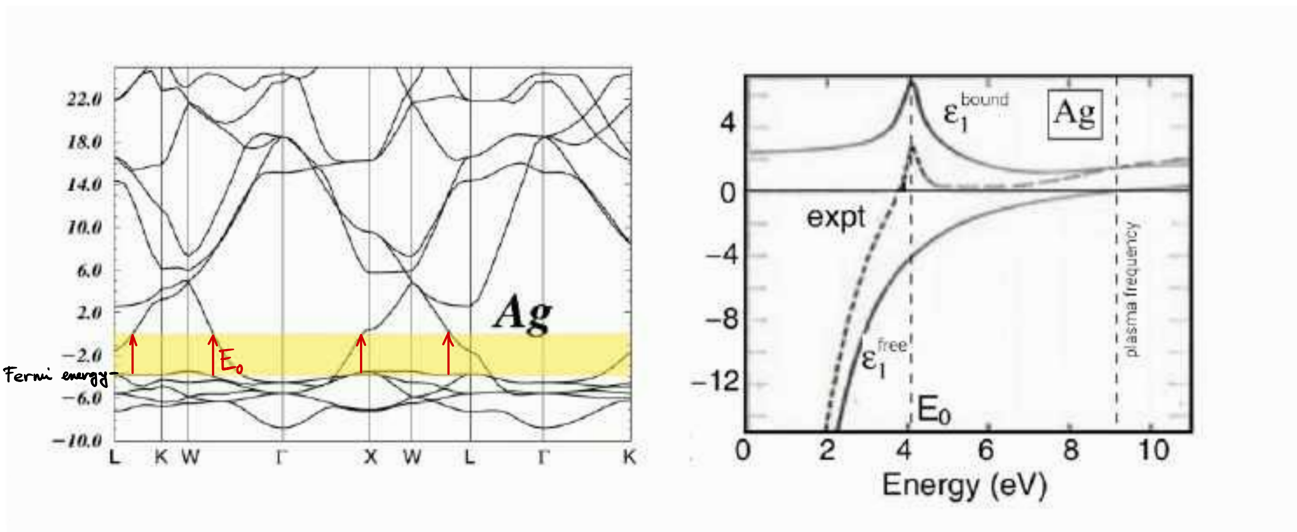


Illustration of the general behavior of the real, $\varepsilon_1(\omega)$ (cyan curves), and imaginary, $\varepsilon_2(\omega)$ (purple curves), parts of the dielectric function with frequency ω in units of the plasma frequency ω_p, for the free-electron case, $\varepsilon^{(f)}(\omega)$ (top-left panel) and the bound-electron case, $\varepsilon^{(b)}(\omega)$ (top-right panel). The bottom figure shows a case where the contributions of the free and bound electrons are added to give the total. In these examples we have taken $\omega_0/\omega_p = 0.6$ for the pole and $\eta/\omega_p = 0.075$.

src. Kaxiras p.290



E_0 – energy of optical transitions between d-states and states at the Fermi level