Chapter 6 Classical light propagation

6.1 The Lorentz oscillator model

The LOM describes the propagation of light in insulators by assuming that matter can be treated as a collection of *atomic*, *molecular* or *vibrational* oscillators. This provides a fundamental explanation for the complex refractive index and all properties that follow from that.

6.1.1 The atomic oscillator

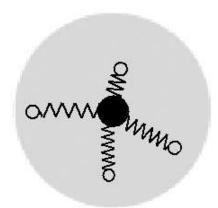


Figure 6.1: Concept of electrons as masses bound to nuclei by spring-like forces. ●

Assume the electrons and the nucleus form a dipole. During oscillations, Fig 6.1, the nucleus remains nearly stationary due to its heavy mass (compared to the electron); therefore, we start by assuming that only a single bound electron oscillates. If the electron has mass m_0 and the 'spring' constant is K_s the natural frequency is:

$$\omega_0 = \sqrt{\frac{K_s}{m_0}} \text{ (rad/s)}. \tag{6.1}$$

Typical frequencies are 10^{15} - 10^{16} Hz (visible – UV). If K_s depends on the direction of vibration, then the material is *optically anisotropic*. The atomic oscillation produces a time varying dipole moment in addition to any pre-existing static atomic dipole moment.

Dipole oscillations lag the applied driving optical field giving rise to delayed re-emission and reduced phase velocity for transmitted light (thus giving a refractive index > 1).

6.2 Dielectric Constant in the Lorentz Model

The magnitude of the time varying dipole moment in the atomic oscillator model is given by Eq. (6.2):

$$p(t) = -ex(t) \tag{6.2}$$

where x(t) is the displacement from the electron's equilibrium position. For one dipole, treated as a damped harmonic oscillator, the equation of motion is Eq.(6.3):

$$m_0 \frac{d^2x}{dt^2} = -m_0 \gamma \frac{dx}{dt} - m_0 \omega_0^2 x - eE(t). \tag{6.3}$$

The three terms on the right hand side are a friction-like force with damping γ , the restoring force, and the optical driving force respectively.

The time dependence of the driving optical electric field is:

$$E(t) = E_0 \cos(\omega t) = E_0 \Re e \left(\exp(-i\omega t) \right) \tag{6.4}$$

and hence we look for solutions of the form

$$x(t) = X_0 \Re e \left(\exp(-i\omega t) \right). \tag{6.5}$$

Any phase difference between the driving field and x is included by allowing X_0 to be complex. We start from Eq.(6.6):

$$E(t) = E_0 \exp(-i\omega t)$$

$$x(t) = X_0 \exp(-i\omega t)$$
(6.6)

Substituting into the equation of motion Eq.(6.3) we get:

$$-m_0\omega^2(X_0e^{-i\omega t}) - im_0\gamma\omega(X_0e^{-i\omega t}) + m_0\omega_0^2(X_0e^{-i\omega t}) = -eE_0e^{-i\omega t}.$$

The solution for X_0 is:

$$X_0 = \frac{-eE_0/m_0}{\omega_0^2 - \omega^2 - i\gamma\omega}. (6.7)$$

If there are N oscillators per unit volume, the resulting induced polarisation of the medium is then:

$$P_{resonant} = Np = -Ne X_0 = \frac{Ne^2}{m_0} \frac{1}{(\omega_0^2 - \omega^2 - i\gamma\omega)} E_0$$
 (6.8)

and the electric displacement D is (when a medium is present):

$$D = \varepsilon_0 E + P. \tag{6.9}$$

We can split the polarization into a non-resonant background term (perhaps due to other oscillators with resonances far from the frequency of the one that is our focus) and the resonant term just calculated for a single type of oscillator:

$$D = \varepsilon_0 E + P_{background} + P_{resonant} \tag{6.10}$$

The background polarisation must arise from some background electric susceptibility χ_b :

$$D = \varepsilon_0 E + \varepsilon_0 \chi_b E + P_{resonant} = \varepsilon_r \varepsilon_0 E. \tag{6.11}$$

Assembling this all together, we find:

$$arepsilon_r(\omega) = 1 + \chi_b + rac{Ne^2}{arepsilon_0 m_0} \, rac{1}{(\omega_0^2 - \omega^2 - i\gamma\omega)}.$$
 (6.12)

Now we can extract the real (ε_1) and imaginary (ε_2) parts of the dielectric function, and these are plotted in Fig 6.2:

$$arepsilon_{1}(\omega)=1+\chi_{b}+rac{Ne^{2}}{arepsilon_{0}m_{0}}~rac{\omega_{0}^{2}-\omega^{2}}{\left(\omega_{0}^{2}-\omega^{2}
ight)^{2}+\left(\gamma\omega
ight)^{2}}$$
 (6.13)

$$arepsilon_2(\omega) = rac{Ne^2}{arepsilon_0 m_0} \; rac{\gamma \omega}{\left(\omega_0^2 - \omega^2\right)^2 + \left(\gamma \omega\right)^2}$$
 (6.14)

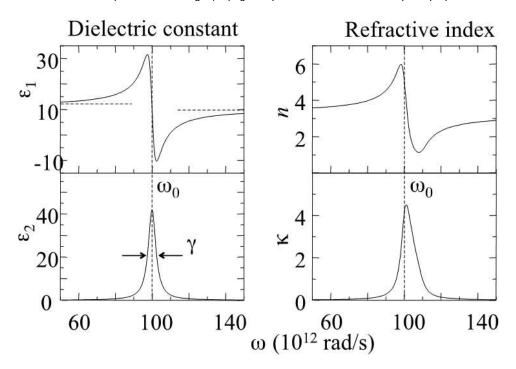


Figure 6.2: Dielectric properties of the Lorentz oscillator. •

The low (static ε_{st}) and high frequency (ε_{∞}) limits are:

$$arepsilon_r(0) \equiv arepsilon_{st} = 1 + \chi_b + rac{Ne^2}{arepsilon_0 m_0 \omega_0^2}$$
 (6.15)

$$\varepsilon_r(\infty) \equiv \varepsilon_\infty = 1 + \chi_b \tag{6.16}$$

6.2.1 Notable features

There is clearly a resonance in ε_2 at $\omega=\omega_0$. It has a full width at half maximum equal to γ (ε_2 is half its maximum value when $\gamma=\omega_0\pm\gamma/2$ – see Problem sheet 2).

Across a resonance region, there is a step change in ε_1 (and also n). Its size is determined by N and ω_0 and it affects a frequency range much wider than the absorption peak.

 ε_1 and n are higher on the low frequency (long wavelength) side of a resonance then on high frequency (short wavelength) side.

6.3 Molecular oscillators

In a polar medium, the electron charge cloud of some or all of the the bonds sits closer to one atom type than the other(s). Ionic molecules are very polar; purely covalent materials, in which identical atoms share electrons, are not polar.

The analysis is same as for the atomic oscillator. ω_0 will be lower because the oscillating mass (reduced mass $\mu=Mm/(M+m)$) is larger than m_0 by a factor ~ 10^4 – 10^5 . Typically $\omega_0\sim 10^{12}-10^{14}$ Hz (near-infrared to far infrared).

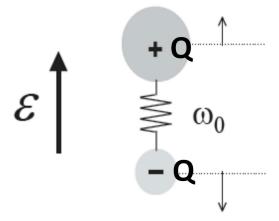


Figure 6.3: Molecular oscillator: a polar molecule in which the atoms are positively and negatively charged. ●

Some gases and most organic compounds can be characterised by the frequencies of their infrared absorption peaks.

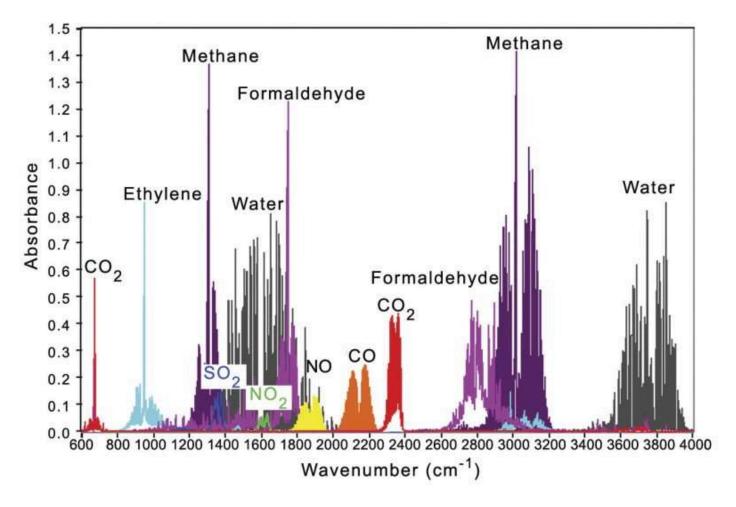


Figure 6.4: IR absorbance of various gases: every sharp line is a real, distinct spectral feature. •