Propagation of Electromagnetic Waves in Continuous Media

Stefan Zollner
Department of Physics
New Mexico State University
December 18, 2018

Contents

1   Scalar and vector waves

A **sinusoidal scalar traveling wave** as a function of **position** $\vec{r}$ and **time** t

$$s\left(\vec{r}, t\right) \;=\; A\cos\left(\vec{k}\cdot\vec{r} - \omega t + \phi\right) \tag{1.1}$$

described by an **amplitude** A, **wave vector** $\vec{k}$, **angular frequency** ω, and **phase** ϕ has an infinite duration and spatial extension. It is difficult to plot or to use in numerical calculations. A more compact mathematical form is preferred. This can be achieved by Fourier series or Fourier transforms.

Similarly to a scalar wave, we can write a **vector wave** in components as

$$\vec{E}\left(\vec{r}, t\right) \;=\; \begin{pmatrix} E_{0x}\cos\left(\vec{k}\cdot\vec{r} - \omega t + \phi\right) \\ E_{0y}\cos\left(\vec{k}\cdot\vec{r} - \omega t + \phi\right) \\ E_{0z}\cos\left(\vec{k}\cdot\vec{r} - \omega t + \phi\right) \end{pmatrix} \;=\; \vec{E}_0\cos\left(\vec{k}\cdot\vec{r} - \omega t + \phi\right), \tag{1.2}$$

where the amplitude is now a **vector** with three components $\vec{E}_0 = (E_{0x}, E_{0y}, E_{0z})$.

Problems:

1.1. Show that the scalar wave in Eq. (1.1) is periodic in time with period $T = 2\pi/\omega$.
1.2. The scalar wave in Eq. (1.1) is also periodic in real space with wavelength $\vec{\lambda}$, written as a vector. Find the relationship between $\vec{\lambda}$ and $\vec{k}$.
1.3. A scalar s is defined as $s = \vec{a}\cdot\vec{b}$. A coordinate transformation defined by a matrix A transforms the unit vectors $\vec{i}$, $\vec{j}$, and $\vec{k}$ into a different set of right-handed unit vectors. Show that the scalar s is invariant under this coordinate transformation.

2   Fourier Series of Periodic Functions

A (real-valued scalar) function $f(t)$ is called **periodic** with **period** T, if $f(t) = f(t+T)$ for all values of t. We see that the scalar wave in Eq. (1.1) is periodic with period $T = 2\pi/\omega$.

A periodic function $f(t)$ with period T can be written as (Jackson 1975, 2.36-37)

$$f(t) \;=\; \frac{1}{2}A_0 + \sum_{m=1}^{\infty}\left[A_m\cos\left(\frac{2\pi m t}{T}\right) + B_m\sin\left(\frac{2\pi m t}{T}\right)\right] \tag{2.1}$$

or

$$f(t) \;=\; \frac{1}{2}A_0 + \sum_{m=1}^{\infty}\left[A_m\cos\left(m\omega t\right) + B_m\sin\left(m\omega t\right)\right] \tag{2.2}$$

with **Fourier coefficients**

$$A_m \;=\; \frac{2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} f(t)\cos\left(\frac{2\pi m t}{T}\right)dt \tag{2.3}$$

$$B_m \;=\; \frac{2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} f(t)\sin\left(\frac{2\pi m t}{T}\right)dt \tag{2.4}$$

or in terms of the angular frequency ω

$$A_m \;=\; \frac{\omega}{\pi}\int_{-\frac{\pi}{\omega}}^{\frac{\pi}{\omega}} f(t)\cos\left(m\omega t\right)dt \tag{2.5}$$

$$B_m \;=\; \frac{\omega}{\pi} \int\limits_{-\frac{\pi}{\omega}}^{\frac{\pi}{\omega}} f(t) \sin(m\omega t)\, dt \tag{2.6}$$

In plain English, Eq. (2.2) means that any periodic function with period T and angular frequency ω can be writen as a sum of its overtones. This is also called **harmonic analysis**.

It is inconvenient that the Fourier series written above have two terms (sines and cosines) and two sets of coefficients. The equations can be simplified by moving to complex numbers. If we remember that

$$\exp(-i\omega t) \;=\; \cos(\omega t) - i\sin(\omega t), \tag{2.7}$$

then we can show that the Fourier series becomes

$$f(t) \;=\; \sum_{m=-\infty}^{+\infty} c_m \exp(-im\omega t) \tag{2.8}$$

with Fourier coefficients (**check !**)

$$c_m \;=\; \frac{\omega}{\pi} \int\limits_{-\frac{\pi}{\omega}}^{\frac{\pi}{\omega}} f(t) \exp(im\omega t)\, dt \;=\; \begin{cases} \frac{A_0}{2}; & m = 0 \\ \frac{1}{2}(A_m + iB_m); & m > 0 \\ \frac{1}{2}(A_{-m} - iB_{-m}); & m < 0 \end{cases} \tag{2.9}$$

Since the function $f(t)$ is a real function (any measurable physical quantity must be real!), the series (2.8) is not really a complex function. All imaginary terms in this series **must** cancel (not individually, but after summation). The Fourier coefficients c_m are only a mathematical definition and not physical quantities. Therefore, the Fourier coefficients are usually complex quantities.

Note: Following the usual ellipsometric convention (see also Born & Wolf, Jackson 1975, etc), we use a minus-sign in the exponential containing the time t. This is different from some math texts. The significance of this choice will be explained later.

Problems:

2.1. A scalar function $f(t)$ is called **even**, if $f(t) = f(-t)$. It is called **odd**, if $f(t) = -f(-t)$. What can you say about the Fourier coefficients A_m and B_m of even and odd functions.

2.2. Use the form of the coefficients c_m in Eq. (2.9) and substitute into Eq. (2.8). Can you recover the Fourier coefficients A_m and B_m in Eqs. (2.3) and (2.4)? (Let me know if you find a mistake!)

2.3. What can you say about the Fourier coefficients c_m for even and odd functions $f(t)$?

2.4. Solve the following integrals for arbitrary integers m_1 and m_2:

$$\frac{\omega}{\pi} \int\limits_{-\frac{\pi}{\omega}}^{\frac{\pi}{\omega}} \cos(m_1\omega t)\cos(m_2\omega t)\, dt \;=\; ? \tag{2.10}$$

$$\frac{\omega}{\pi} \int\limits_{-\frac{\pi}{\omega}}^{\frac{\pi}{\omega}} \sin(m_1\omega t)\sin(m_2\omega t)\, dt \;=\; ? \tag{2.11}$$

$$\frac{\omega}{\pi} \int\limits_{-\frac{\pi}{\omega}}^{\frac{\pi}{\omega}} \sin(m_1\omega t)\cos(m_2\omega t)\, dt \;=\; ? \tag{2.12}$$

The functions $\sqrt{\frac{\omega}{\pi}}\cos(m\omega t)$ and $\sqrt{\frac{\omega}{\pi}}\sin(m\omega t)$ (where m is an integer) form an orthonormal basis set for the infinite-dimensional vector space of periodic functions with period T (Jackson 1975, Sec. 2.8).

3

2.5. Show that the function $f(t)$ in Eq. (2.8) is real, i.e., equal to its complex conjugate.

2.6. Check out the article on Fourier series in wikipedia and calculate the first few terms in the Fourier series for a square wave and a sawtooth wave (stop reading after example 1). Many compilations of mathematical tables (such as Bronstein-Semendjajew 1979) list Fourier series expansions of common functions.

3   Fourier Transforms of Non-periodic Functions

If the function $f(t)$ is not periodic, then the period T becomes infinite and the frequency spacing ω between overtones becomes very small. Instead of needing a series of discrete overtones with spacing ω (as for finite period T), we now need a continuous set of angular frequencies ω. The Fourier series (2.8) becomes a **Fourier integral** (Jackson 1975, 2.44)

$$f(t) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega) \exp(-i\omega t)\, d\omega. \tag{3.1}$$

The function $F(\omega)$ is called the **Fourier transform** of $f(t)$

$$F(\omega) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) \exp(i\omega t)\, dt. \tag{3.2}$$

I have written the Fourier transform (3.2) and the **inverse Fourier transform** (3.1) with a symmetric prefactor $\frac{1}{\sqrt{2\pi}}$. This notation can vary (Jackson 1975, 6.55-56). For any function $f(t)$ describing a physical quantity, the imaginary terms in the inverse Fourier transform (3.1) must cancel to make the function real-valued. The Fourier transform $F(\omega)$ may be complex, since it is not a physical quantity. Just like the time t, the angular frequency ω is a real quantity in these transforms.

The **orthogonality and completeness relations** are now (Jackson 1975, 2.46-47)

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left[i\left(\omega - \omega'\right) t\right] dt \;=\; \delta\left(\omega - \omega'\right) \tag{3.3}$$

and

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left[i\omega\left(t - t'\right)\right] d\omega \;=\; \delta\left(t - t'\right), \tag{3.4}$$

where $\delta(t)$ is the Kronecker δ-function. These integrals (3.3) and (3.4) are not to be taken literally, since the δ-function is not a real function. These equations only become meaningful mathematically within the theory of functional analysis. Only integrals containing the δ-function as a **kernel** become meaningful. The functions $\frac{1}{\sqrt{2\pi}} \exp(i\omega t)$ form an orthonormal basis of a **Hilbert space** of functions.

Problems:

3.1. The **convolution** $(f * g)(t)$ of two functions $f(t)$ and $g(t)$ is defined by

$$(f * g)(t) \;=\; \int_{-\infty}^{\infty} f(t')\, g(t - t')\, dt'. \tag{3.5}$$

Show that the Fourier transform of the convolution of two functions $f(t)$ and $g(t)$ is equal to the product of their Fourier transforms $F(\omega)$ and $G(\omega)$ (up to a factor of $\sqrt{2\pi}$), i.e.,

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (f * g)(t) \exp(i\omega t)\, dt \;=\; \sqrt{2\pi} F(\omega)\, G(\omega). \tag{3.6}$$

4

3.2. Can we choose a normalization factor other than $\sqrt{2\pi}$ in the Fourier transform to get rid of the prefactor $\sqrt{2\pi}$ in the convolution theorem?

3.3. If $F(\omega)$ is the Fourier transform of $f(t)$, then the Fourier transform of the derivative $f'(t)$ is $i\omega F(\omega)$. In other words,

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f'(t) \exp(i\omega t)\, dt = i\omega F(\omega). \tag{3.7}$$

3.4. If $F(\omega)$ is the Fourier transform of $f(t)$, show that $F(-\omega) = \bar{F}(\omega)$ (i.e., the complex conjugate of $F(\omega)$).

4   Fourier Transforms and Fourier Series in Multiple Dimensions

The Fourier transforms described in Sec. 3 are written in one dimension. An example for this is the transform from time into frequency space. We can also transform scalar or vector functions in real space and move into wave vector space. (In quantum mechanics or solid-state physics, this would be called momentum space or reciprocal space.)

A scalar field $s(\vec{r})$ in a **crystal (Bravais lattice)** is called periodic if $s\left(\vec{r}+\vec{R}\right) = s(\vec{r})$ for all **Bravais lattice vectors** $\vec{R} = u\vec{a} + v\vec{b} + w\vec{c}$ with integral coefficients u, v, and w and primitive lattice translations $\vec{a}$, $\vec{b}$, and $\vec{c}$ spanning the unit cell $V = \vec{a} \cdot \left(\vec{b} \times \vec{c}\right)$. In this case (Ashcroft & Mermin 1976, Appendix D), the three-dimensional Fourier series is given by a sum over all **reciprocal lattice vectors** $\vec{G} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$ (with real-valued components)

$$s(\vec{r}) = \sum_{\vec{G}} s_{\vec{G}} \exp\left(i\vec{G} \cdot \vec{r}\right), \tag{4.1}$$

where

$$\vec{a}^* = \frac{2\pi}{V}\left(\vec{b} \times \vec{c}\right), \quad \vec{b}^* = \frac{2\pi}{V}\left(\vec{c} \times \vec{a}\right), \quad \text{and} \quad \vec{c}^* = \frac{2\pi}{V}\left(\vec{a} \times \vec{b}\right) \tag{4.2}$$

and the Fourier coefficients are given by

$$s_{\vec{G}} = \frac{1}{V} \int_C s(\vec{r}) \exp\left(-i\vec{G} \cdot \vec{r}\right) d^3\vec{r}. \tag{4.3}$$

The integral is over the **primitive cell** C spanned by $\vec{a}$, $\vec{b}$, and $\vec{c}$ with volume V. Compare the one-dimensional case in Eq. (2.8), which is the same except for a different sign and for a factor of $2^3 = 8$. (For a periodic time-dependent function with period T, the unit cell volume is $V = T = 2\pi/\omega$ and $2\pi/V = \omega$ is the reciprocal space unit.) This formalism can also be applied to functions periodic in reciprocal space. As always, the imaginary terms in the series (4.1) must cancel if the scalar field $s(\vec{r})$ is a real-valued physical quantity.

The same equations apply to a periodic vector field

$$\vec{E}(\vec{r}) = \sum_{\vec{G}} \vec{E}_{\vec{G}} \exp\left(i\vec{G} \cdot \vec{r}\right), \tag{4.4}$$

where the Fourier coefficients are given by

$$\vec{E}_{\vec{G}} = \frac{1}{V} \int_C \vec{E}(\vec{r}) \exp\left(-i\vec{G} \cdot \vec{r}\right) d^3\vec{r}. \tag{4.5}$$

As always, the imaginary terms in the series (4.4) must cancel if the vector field $\vec{E}(\vec{r})$ is a real-valued physical quantity.

Now let us turn to the Fourier transforms for non-periodic scalar and vector fields. The three-dimensional Fourier integral for a scalar field $s(\vec{r})$ becomes

$$s(\vec{r}) \;=\; \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} S(\vec{k}) \exp\left(i\vec{k}\cdot\vec{r}\right) d^3\vec{k}. \tag{4.6}$$

The function $S\left(\vec{k}\right)$ is called the **Fourier transform** of $s(\vec{r})$

$$S(\vec{k}) \;=\; \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} s(\vec{r}) \exp\left(-i\vec{k}\cdot\vec{r}\right) d^3\vec{r}. \tag{4.7}$$

Similar equations hold for non-periodic vector fields $\vec{E}(\vec{r})$

$$\vec{E}(\vec{r}) \;=\; \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \vec{E}(\vec{k}) \exp\left(i\vec{k}\cdot\vec{r}\right) d^3\vec{k} \tag{4.8}$$

with the Fourier transform defined by

$$\vec{E}(\vec{k}) \;=\; \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \vec{E}(\vec{r}) \exp\left(-i\vec{k}\cdot\vec{r}\right) d^3\vec{r}. \tag{4.9}$$

As always, the imaginary terms in the inverse Fourier transforms (4.6) and (4.8) must cancel if the scalar field $s(\vec{r})$ and the vector field $\vec{E}(\vec{r})$ are real-valued physical quantities. The vectors $\vec{r}$ and $\vec{k}$ also have real components.

5   Maxwell's Equations in Vacuum (Microscopic)

In mechanics, our goal is to determine the position $\vec{r}$ of a particle with mass m exposed to a net force $\vec{F}$, given the initial position and velocity. The equation of motion is Newton's second law: $\vec{F} = m\ddot{\vec{r}}$. In the theory of electricity and magnetism, the **electric field strength** $\vec{E}$ and the **magnetic field strength** $\vec{H}$ need to be determined using initial or boundary conditions for a given **charge density** ρ and **current density** $\vec{j}$. Both fields $\vec{E}$ and $\vec{H}$ are vector fields and depend on position and time, but they can be Fourier-transformed and then become functions of wave vector $\vec{k}$ and angular frequency ω. Maxwell's equations take the place of Newton's second law. (The definition of the magnetic field strength $\vec{H}$ follows Serway 1990, Sec. 30.9. See also Holm 1991. This allows a symmetric treatment of the dielectric and magnetic susceptibilities involving the microscopic pair of quantities $\vec{E}$ and $\vec{H}$ turning into $\vec{D}$ and $\vec{B}$ in the macroscopic case.)

For completeness, we also define the **dielectric displacement** $\vec{D}$ and the **magnetic field** $\vec{B}$ (also known as the **magnetic flux density**)

$$\vec{D} \;=\; \epsilon_0 \vec{E} \tag{5.1}$$
$$\vec{B} \;=\; \mu_0 \vec{H}. \tag{5.2}$$

Let's keep in mind that these expressions (5.1-5.2) are only valid in vacuum and need to be modified inside a continuous medium.

In differential form, the general microscopic form of Maxwell's equations is

$$\text{Gauss' law (electric field)} \quad \vec{\nabla}\cdot\vec{E} = \frac{\rho}{\epsilon_0} \tag{5.3}$$

6

$$\text{Gauss' law (magnetic field)} \quad \vec{\nabla} \cdot \vec{H} = \quad 0 \tag{5.4}$$

$$\text{Faraday's law} \quad \vec{\nabla} \times \vec{E} = \quad -\mu_0 \frac{\partial \vec{H}}{\partial t} \tag{5.5}$$

$$\text{Ampere's law} \quad \vec{\nabla} \times \vec{H} = \quad \vec{j} + \epsilon_0 \frac{\partial \vec{E}}{\partial t}, \tag{5.6}$$

where ϵ_0 is the **permittivity of free space** and μ_0 the **permeability of free space**.

The first equation is **Coulomb's law** and implies that the electric field strength from a point charge drops off like the square of the distance. The second equation states that there are no magnetic charges. **Faraday's law** states that a flux change causes an induced voltage. (There is no magnetic current, because there are no magnetic charges.) **Ampere's law** states that the magnetic field strength curls around the current. We can apply **Gauss' theorem** and **Stokes' theorem** to convert these equations into their integral form (but this is not necessary here).

There's a few other things to note about Maxwell's equations: They are linear in the fields $\vec{E}$ and $\vec{H}$, they are first order in space coordinates and time, and they have constant coefficients ϵ_0 and μ_0. (Actually, if we choose different units, the speed of light c is the only parameter in these equations. The speed of light couples the electric and magnetic field strenghts.) However, these equations are inhomogeneous: The charge density ρ and the current density $\vec{j}$ are the inhomogeneous sources. Because of the linearity of the equations, if the systems $\left\{\vec{E}_1, \vec{H}_1, \rho_1, \vec{j}_1\right\}$ and $\left\{\vec{E}_2, \vec{H}_2, \rho_2, \vec{j}_2\right\}$ solve Maxwell's equations, then $\left\{\vec{E}_1 + \vec{E}_2, \vec{H}_1 + \vec{H}_2, \rho_1 + \rho_2, \vec{j}_1 + \vec{j}_2\right\}$ is also a solution. This linearity allows us to Fourier-transform Maxwell's equations. Because of linearity, the integrals commute with the partial derivatives. Finally, we see that the electric and magnetic field strengths $\vec{E}$ and $\vec{H}$ are only coupled through the partial time derivatives. Therefore, electrostatics and magnetostatics are independent and the static fields don't mix. The electric and magnetic field strengths $\vec{E}$ and $\vec{H}$ are only coupled, once we consider dynamic (time-dependent) effects, for example in the theory of the propagation of electromagnetic waves.

Since we are interested in the propagation of electromagnetic waves, we don't have to worry about free charges (ρ=0) and currents flowing through a wire ($\vec{j} = 0$). Therefore, Maxwell's equations in vacuum read as follows (Jackson 1975, 7.1):

$$\text{Gauss' law (electric field)} \quad \vec{\nabla} \cdot \vec{E} = \quad 0 \tag{5.7}$$
$$\text{Gauss' law (magnetic field)} \quad \vec{\nabla} \cdot \vec{H} = \quad 0 \tag{5.8}$$

$$\text{Faraday's law} \quad \vec{\nabla} \times \vec{E} = \quad -\mu_0 \frac{\partial \vec{H}}{\partial t} \tag{5.9}$$

$$\text{Ampere's law} \quad \vec{\nabla} \times \vec{H} = \quad \epsilon_0 \frac{\partial \vec{E}}{\partial t}. \tag{5.10}$$

While the current density $\vec{j}$ vanishes, we note that we still need to deal with the displacement current density on the right hand side of Ampere's law. The speed of light c is defined by

$$c = \frac{1}{\sqrt{\epsilon_0 \mu_0}}. \tag{5.11}$$

Maxwell's equations are now truly homogeneous without any source terms. Because of the linearity of the equations, if the systems $\left\{\vec{E}_1, \vec{H}_1\right\}$ and $\left\{\vec{E}_2, \vec{H}_2\right\}$ solve the homogeneous Maxwell's equations, then $\left\{\vec{E}_1 + \vec{E}_2, \vec{H}_1 + \vec{H}_2\right\}$ is also a solution.

Problems:

5.1. Derive the **wave equations** (Holm 1991, Jackson 1975)

$$\vec{\nabla}^2 \vec{E} - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} = \quad 0 \quad \text{and} \tag{5.12}$$

$$\vec{\nabla}^2 \vec{H} - \frac{1}{c^2} \frac{\partial^2 \vec{H}}{\partial t^2} \;=\; 0 \tag{5.13}$$

from Maxwell's equations in vacuum. See Good & Nelson 1971, 4.7.

5.2. Show the following: If the systems $\left\{\vec{E}_1, \vec{H}_1, \rho_1, \vec{j}_1\right\}$ and $\left\{\vec{E}_2, \vec{H}_2, \rho_2, \vec{j}_2\right\}$ solve Maxwell's equations, then $\left\{\vec{E}_1 + \vec{E}_2, \vec{H}_1 + \vec{H}_2, \rho_1 + \rho_2, \vec{j}_1 + \vec{j}_2\right\}$ is also a solution.

5.3. What are the units of the electric and magnetic field strengths $\vec{E}$ and $\vec{H}$ in the MKSA system? The **Poynting vector** is defined as (Serway 1990, 34.23)

$$\vec{S} \;=\; \vec{E} \times \vec{H}. \tag{5.14}$$

What is the direction and the unit of the Poynting vector?

6   Plane Wave Solutions to Maxwell's Equations in Vacuum

As stated before, the purpose of Maxwell's equations is to determine the electric and magnetic field strengths $\vec{E}(\vec{r}, t)$ and $\vec{H}(\vec{r}, t)$ for a given charge and current density. Maxwell's equations are linear and therefore the integrals in the Fourier transformed fields commute with the differential operators in Maxwell's equations. Let's Fourier transform the electric field strength $\vec{E}(\vec{r}, t)$ in all four dimensions (position $\vec{r}$ and time t). The resulting Fourier transforms are given by

$$\vec{E}\left(\vec{k}, \omega\right) \;=\; \left(\frac{1}{2\pi}\right)^2 \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \vec{E}(\vec{r}, t) \exp\left[-i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right] d^3\vec{r}\, dt \quad \text{and} \tag{6.1}$$

$$\vec{E}(\vec{r}, t) \;=\; \left(\frac{1}{2\pi}\right)^2 \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \vec{E}\left(\vec{k}, \omega\right) \exp\left[i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right] d^3\vec{k}\, d\omega \tag{6.2}$$

with a corresponding expression for the magnetic field strength $\vec{H}(\vec{r}, t)$.

We note that the exponential phase has the opposite sign in the Fourier transform (6.1) and the inverse Fourier transform (6.2). How we choose this phase (if the minus sign appears in the Fourier transform or in the inverse transform) is convention. In the Nebraska convention for ellipsometric measurements as modified by Aspnes (Muller 1969, Holm 1991, Humlíček 2005, Jackson 1975), Eq. (6.2) with the negative time dependence factor is the preferred choice. The form of the exponential in Eq. (6.1) with the minus sign applied to time is also the preferred choice for a quantum-mechanical wave packet to ensure that the kinetic energy of a free particle is positive (Holm 1991). This choice has profound consequences on the sign of the imaginary part of the dielectric constant (related to the extinction coefficient). Unfortunately, the positive sign of the time-dependence is almost universally in use in electrical engineering. This makes it difficult to transition from the optical to the microwave regime, if different conventions are used. Finally, we note that the terms involving time and space coordinates have opposite signs in the usual convention. (In a one-dimensional case with the wave moving along the z-direction, the wave moves towards increasing z with increasing time t.)

A **plane wave** $\vec{E}\left(\vec{k}, \omega\right)$ with wave vector $\vec{k}$ and angular frequency ω is a δ-function in wave vector and angular frequency space and thus all four integrals collapse. The electric field strength for a plane wave looks like this:

$$\vec{E}(\vec{r}, t) \;=\; \vec{E}_0 \exp\left[i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right]. \tag{6.3}$$

There is a similar equation for the magnetic field strength $\vec{H}(\vec{r}, t)$ of a plane wave:

$$\vec{H}(\vec{r}, t) \;=\; \vec{H}_0 \exp\left[i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right]. \tag{6.4}$$

8

Both $\vec{E}_0$ and $\vec{B}_0$ are vectors with complex coefficients, but they do not depend on the space and time coordinates $\vec{r}$ and t.

Unfortunately, plane waves are not physical solutions to Maxwell's equations for two reasons: First, because the electric and magnetic field strengths are not real-valued, but complex quantities. Second, the fields are δ-functions in wave vector and frequency space, with infinitely sharp frequencies and wave vectors. To form a physical solution, we must do two things. First, we form a wave packet with smoothly varying envelope functions $\vec{E}\left(\vec{k}, \omega\right)$ and $\vec{H}\left(\vec{k}, \omega\right)$ in frequency and wave vector space. A Gaussian superposition is very popular, because it resembles the output of a well-tuned laser. Second, we add the complex conjugate wave (terms with negative frequencies and wave vectors) to achieve real-valued smoothly varying solutions $\vec{E}\left(\vec{r}, t\right)$ and $\vec{H}\left(\vec{r}, t\right)$. While they are not physical solutions, plane waves form an orthonormal basis of the Hilbert space containing all solutions to Maxwell's equations. They are also very easy to deal with from a mathematical viewpoint.

For a plane wave in Eqs. (6.3-6.4), the phase of the wave is a well-defined quantity for any given time or position. We say that the **coherence length** of a plane wave is infinite. If we form a Gaussian wave packet, then the frequency spread of the wave causes an uncertainty of the phase for times $t \neq 0$ or away from the origin. The phase is defined reasonably well only within one coherence length of the origin. At distances further away, only the magnitude of the wave (i.e., its intensity) is well-defined. Therefore, interference effects of two waves with the same frequency can only be observed if the two waves are less than one coherence lenght apart (i.e., if the path difference is less than a coherence length). In this case, we add electric and magnetic field strenghts. For path differences much greater than one coherence length, we add intensities, not the field amplitudes.

The Fourier transform equations (6.1) and (6.2) say that any electric field can be constructed by superposition of plane waves (orthogonality and completeness). If we can show that the plane waves (6.3-6.4) are a solution to Maxwell's equations (5.7-5.10), then we can form the general solution by superposition.

Substitution of the electric and magnetic fields (6.3) and (6.4) into Maxwell's equations (5.7-5.10) in vacuum yields the following (see Good & Nelson 1971, page 384): (CHECK!)

$$\text{Gauss' law (electric field)} \quad \vec{k} \cdot \vec{E}_0 = \quad 0 \tag{6.5}$$

$$\text{Gauss' law (magnetic field)} \quad \vec{k} \cdot \vec{H}_0 = \quad 0 \tag{6.6}$$

$$\text{Faraday's law} \quad \vec{k} \times \vec{E}_0 = \quad \omega \mu_0 \vec{H}_0 \tag{6.7}$$

$$\text{Ampere's law} \quad \vec{k} \times \vec{H}_0 = \quad -\omega \epsilon_0 \vec{E}_0. \tag{6.8}$$

Therefore, plane waves indeed solve Maxwell's equations in vacuum, but only under certain conditions (6.5-6.8) for the frequency and wave vector. The first two equations state that the electric and magnetic fields for an electromagnetic wave with non-vanishing amplitudes are perpendicular to the wave vector. We therefore say that electromagnetic waves are **transverse waves**, because the disturbance is perpendicular to the direction of propagation. The last two equations state that the electric and magnetic field strengths are also perpendicular to each other. The unit vectors for the fields and the direction of propagation form a right-handed coordinate system. Finally, by substituting Faraday's law (6.7) into Ampere's law (6.8), we obtain the equivalent of the wave equation (5.12): (CHECK !)

$$k^2 = \frac{\omega^2}{c^2} \tag{6.9}$$

This is called a **dispersion relation**, because it contains an expression between the wave vector $\vec{k}$ and the angular frequency ω. This dispersion relation defines the speed of the wave (in this case the speed of light).

Looking at the simplicity of Maxwell's equations and the wave equation for a plane wave, you will understand why we went through the trouble of defining the Fourier transformation and the inconvenience of a complex-valued solution in the form of a plane wave.

Faraday's Law and Ampere's Law allow us to compare the magnitude of the electric and magnetic field strengths. We find that (Fox, A.36-37)

$$E_0 = \sqrt{\frac{\mu_0}{\epsilon_0}} H_0 = Z_0 H_0. \tag{6.10}$$

The quantity $Z_0 = 377 \ \Omega$ is called the impedance of vacuum.

Problems:

6.1. For an electric field

$$\vec{E}(\vec{r},t) = \vec{E}_0 \exp\left[i\left(\vec{k} \cdot \vec{r} - \omega t\right)\right] \tag{6.11}$$

show that (CHECK !)

$$\vec{\nabla} \cdot \vec{E}(\vec{r},t) = i\vec{k} \cdot \vec{E} \tag{6.12}$$

$$\vec{\nabla} \times \vec{E}(\vec{r},t) = i\vec{k} \times \vec{E} \tag{6.13}$$

$$\frac{\partial \vec{E}(\vec{r},t)}{\partial t} = -i\omega \vec{E} \tag{6.14}$$

$$\vec{\nabla}^2 \vec{E}(\vec{r},t) = -k^2 \vec{E} \tag{6.15}$$

$$\frac{\partial^2 \vec{E}(\vec{r},t)}{\partial t^2} = -\omega^2 \vec{E} \tag{6.16}$$

6.2. Derive the wave equation (6.9) from Faraday's law and Ampere's law in $\vec{k}$-dependent form.

7 Polarized Light in Vacuum; Jones vectors; Stokes parameters

For an electromagnetic wave propagating along the z-direction, let's write the wave vector as $\vec{k} = k\hat{k}$, where k is the magnitude of the wave vector and $\hat{k}$ the unit vector along the z-axis. Gauss' law for plane waves (6.5)-(6.6) forces $E_{0z} = 0$ and $H_{0z} = 0$, another statement of the transverse character of electromagnetic waves. Together with the wave equation (dispersion relation) (6.9), we can write the magnetic field strength $\vec{H}$ as a function of the electric field strength $\vec{E}$:

$$H_{0x} = -\sqrt{\frac{\epsilon_0}{\mu_0}} E_{0y} \tag{7.1}$$

$$H_{0y} = \sqrt{\frac{\epsilon_0}{\mu_0}} E_{0x} \tag{7.2}$$

Therefore, an electromagnetic plane wave is described by the following quantities:

- the direction of propagation (wave vector),
- the angular frequency ω (which defines the magnitude k of the wave vector),
- the magnitudes of the electric field strength perpendicular to the wave vector (which is related to the magnetic field strengths through the equations above).

If we fix the angular frequency ω, the electromagnetic wave is described by only two complex numbers E_{ox} and E_{0y}, i.e., four real quantities. As a function of position coordinate and time, the electric field strength of the wave can be written as a vector with two columns

$$\vec{E}(\vec{r},t) = \begin{pmatrix} E_{0x} \\ E_{0y} \end{pmatrix} \exp\left[i\left(kz - \omega t\right)\right]. \tag{7.3}$$

This wave is known as a *plane wave*, because the electric field strength does not depend on the x and y coordinates. In the xy-plane (where $z=0$), the electric field is

$$\vec{E}(z = 0, t) = \begin{pmatrix} E_{0x} \\ E_{0y} \end{pmatrix} \exp\left(-i\omega t\right). \tag{7.4}$$

10

Keeping in mind that the quantities E_{0x} and E_{0y} are complex numbers, they have an amplitude (real) and a phase. Let's call the (real) magnitude of the electric field E_0 and the *normalized* real amplitudes of the electric field strength in the x and y directions X and Y, respectively. Let's call the corresponding phases Δ_X and Δ_Y. The electric field in the xy-plane then becomes

$$\vec{E}(z=0,t) = E_0 \begin{pmatrix} X \exp(i\Delta_X) \\ Y \exp(i\Delta_Y) \end{pmatrix} \exp(-i\omega t). \tag{7.5}$$

We can easily rewrite this as (see Humlicek 2005, Fujiwara 2007)

$$\vec{E}(z=0,t) = E_0 \begin{pmatrix} X \exp(i\Delta) \\ Y \end{pmatrix} \exp[-i\omega(t-t_0)], \tag{7.6}$$

if $\Delta = \Delta_X - \Delta_Y$ and $t_0 = \Delta_Y/\omega$. The vector

$$\begin{pmatrix} X \exp(i\Delta) \\ Y \end{pmatrix} \tag{7.7}$$

is called the *Jones vector* of the electromagnetic wave. Defining

$$\tan \psi = \frac{X}{Y}, \tag{7.8}$$

the Jones vector can also be written as

$$\begin{pmatrix} \sin\psi \exp(i\Delta) \\ \cos\psi \end{pmatrix}, \tag{7.9}$$

where ψ and Δ are called the *ellipsometric angles*.

For $\Delta = 0$ or $\Delta = \pi$, we obtain *linearly polarized* light. For $\psi = \pi/4$ and $\Delta = \pi/2$ or $\Delta = -\pi/2$, we obtain *circularly polarized* light. In the most general case, where ψ ranges from 0 to $\pi/2$ and Δ ranges from $-\pi$ to π, we obtain *elliptically polarized* light.

Show examples of Jones vectors for linearly and circularly polarized light. Compare Table 3.1 in Fujiwara 2007.

Define Stokes parameters following Section 3.4 in Fujiwara 2007. Introduce Poincare sphere. Discuss totally and partially polarized light. Introduce depolarization.

8 Ellipsometry

In an ellipsometry experiment, we have an incident beam and a detected (reflected) beam, each with an electric field strength with complex amplitude

$$E_0 \begin{pmatrix} X \exp(i\Delta) \\ Y \end{pmatrix}. \tag{8.1}$$

In the experiment, the detected beam was somehow altered (for example by reflection by or transmission through a sample).

Define Jones matrix as relating the Jones vectors for the incident and reflected (or transmitted beam) by a two-by-two matrix with complex coefficients. Off-diagonal elements vanish for isotropic materials, but can be non-zero in case of anisotropy.

Define Mueller matrix as the relationship between incident and reflected (or transmitted) Stokes parameters.

9 Dielectric in a Static Electric and Magnetic Field

After the propagation of electromagnetic waves (i.e., light) in vacuum has been described, we now turn to the response of materials to an electromagnetic field. Before we can discuss the response of materials to time-dependent fields, we must first describe their response to static electric and magnetic fields.

Referring to Fig. 1, we first consider a dielectric exposed to a homogeneous externally applied electric field $\vec{E}_0$. The charges (positively charged nuclei and negatively charged electrons) in the dielectric respond to the external field with small displacements. The positive charges in the material are pulled along the field lines of the applied electric field (shown by solid lines), while negative charges are forced in the opposite direction. The piece of material as a whole is still electrically neutral and the average macroscopic charge density is zero (look inside the green box, for example). However, these small displacements collectively create an induced electric field $\vec{E}_1$ opposite to the applied external field. The electric field lines of the induced electric field (shown by the dashed lines) point from the positive charges to the negative charges. Also, the material has acquired a positive surface charge on the left and a negative surface charge on the right.

The total (local) electric field $\vec{E}$, sometimes called $\vec{E}_{\text{local}}$, is the sum of the applied (external) electric field $\vec{E}_0$ and the induced (depolarizing) electric field $\vec{E}_1$, i.e, $\vec{E} = \vec{E}_0 + \vec{E}_1$ (Nye 1985). The magnitude of the local electric field is usually smaller than that of the external applied field $\vec{E}_0$. This is called screening. (See Fox 2010, Clausius-Mossotti relationship.)
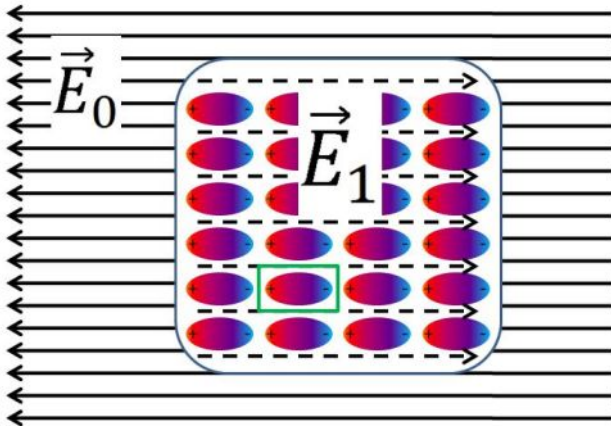

Figure 1: A dielectric material is placed inside a homogeneous static electric field $\vec{E}_0$. The charges (positively charged nuclei and negatively charged electrons) in the dielectric respond to the external field with a small displacement. This displacement creates an induced electric field $\vec{E}_1$ opposite to the applied external field. The total (local) electric field is therefore $\vec{E} = \vec{E}_0 + \vec{E}_1$, which is called screening. The charge displacements create a dipole moment, which is proportional to the local electric field $\vec{E}$. The dielectric polarization is defined as the dipole moment per unit volume.

Each small charge displacement creates an electric dipole. We remember that the magnitude of the **dipole moment** $\vec{p} = q\Delta\vec{r}$ is equal to the distance between the charges times the magnitude of the charge (Young & Freedman 1987, Sec. 21.7). The dipole moment as a vector points from the negative charge to the positive charge. The **dielectric polarization** $\vec{P}$ is defined as the dipole moment per unit volume (average over the green box, for example). Now we are ready to define the dielectric constant and the dielectric displacement.

The **dielectric displacement** $\vec{D}$ for a material is obtained as a sum, including the original electric field (in vacuum) and the dielectric polarization:

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}. \tag{9.1}$$

If the electric field is not too large (below the dielectric breakdown strength of the material) and in the absence of ferroelectric effects (where a non-vanishing dielectric polarization remains even in the absence of an electric field), the dielectric polarization is proportional to the applied electric field. This defines the **dielectric susceptibility** χ_e as

$$\vec{P} = \epsilon_0 \chi_e \vec{E}. \tag{9.2}$$

In the ferroelectric case, this can be generalized as

$$\vec{P} = \vec{P}_r + \epsilon_0 \chi_e \vec{E}, \tag{9.3}$$

where $\vec{P}_r$ is the remanent (ferroelectric) polarization at a vanishing electric field $\vec{E}$.

The **dielectric constant** ϵ is defined by

$$\epsilon = 1 + \chi_e. \tag{9.4}$$

The dielectric displacement can therefore be written as

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P} = \vec{P}_r + \epsilon\epsilon_0 \vec{E} \tag{9.5}$$

as a product involving the dielectric constant and the applied electric field (if $\vec{P}_r$ vanishes).

So far, we have assumed that the charges in the dielectric will move the same distance (create the same magnitude of polarization) regardless of the direction of the applied electric field $\vec{E}$. This is true for isotropic materials. In uniaxial or biaxial crystals, the charges may actually move in a direction different from the applied electric field, because the restoring force inside the crystal varies with direction. Therefore, the induced electric field E_1, the dielectric polarization $\vec{P}$, and also the dielectric displacement $\vec{D}$ may not be parallel to the applied electric field $\vec{E}$. In mathematical terms, the dielectric susceptibility χ_e and the dielectric constant ϵ are not numbers, but 3×3 tensors. This makes calculations more difficult.

Furthermore, a polarization of the medium in a paramagnet can also be caused by an applied magnetic field of strength $\vec{H}$. Examples of such magneto-optical effects are the magneto-optical Faraday effect (in transmission) and Kerr effect (in reflection). Including magneto-electric effects, the displacement is written in an even more general form as (Schubert 2005)

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P} = \vec{P}_r + \epsilon_0 \epsilon \vec{E} + \epsilon_0 \delta \vec{H}. \tag{9.6}$$

The term $\epsilon_0 \delta \vec{H}$ describes the polarization in a paramagnet. In a ferromagnet, the polarization can depend on the magnetization even in the absence of a magnetic field $\vec{H}$. In the ferromagnetic case, the magneto-optical properties of the material are described by off-diagonal elements in the dielectric tensor ϵ (Mansuripur 1995, Schubert 2005).

The ferroelectric remanence $\vec{P}_r$ will vary only slowly with time, especially at optical frequencies, because the charges must be moved across large ferroelectric domains, which takes longer than moving a single charge. Therefore, without loss of generality, we may assume that

$$\frac{\partial \vec{P}_r}{\partial t} = 0. \tag{9.7}$$

Similarly, if the ferroelectric domains are infinitely large, then the spatial derivatives of $\vec{P}_r$ will vanish also, but this is not true across domain walls.

Problems:

9.1. What are the units of $\vec{E}$, $\vec{D}$, $\vec{P}$, χ_ϵ, ϵ_0, and ϵ, in MKSA units?

9.2. A dielectric contains bound charges with charge q and charge density n. We apply a static electric field $\vec{E}$. Assume that the charges respond by moving in the same direction as the field (isotropic model) and that the restoring force is proportional to the displacement with a spring constant $k = m\omega_0^2$ (linear approximation for small electric fields). Show that the static dielectric susceptibility is (Jackson 1975, 4.72)

$$\chi_e = \frac{nq^2}{m\epsilon_0\omega_0^2} = \frac{\omega_P^2}{\omega_0^2}. \tag{9.8}$$

For reasons that will become clear later, the term

$$\omega_P = \sqrt{\frac{nq^2}{m\epsilon_0}} \tag{9.9}$$

is called the **plasma frequency**.

13

9.3. Let's treat an ideal gas as a dielectric. What is the density of molecules at normal temperature and pressure? Each molecule has several types of charges. The nuclei (positive charges) contribute very little, because of the large mass in the denominator. Charges in completely filled (inner) shells contribute very little, because they are bound very tightly and have large values of ω_0. Let's only consider electrons in partially filled shells contributing to molecular bonds. What is the plasma frequency for such a gas (give a range, based on the number of charges per molecule)? Assuming that the resonance wavelength λ_0 is 100 to 300 nm, estimate a range of expected values for the susceptibility of a gas (like hydrogen, oxygen, nitrogen, etc). Compare your result with literature values for the refractive indices of various gases. (See Jackson 1975, Sec. 4.6.)

10 Magnetostatics and Magnetization

While there are no magnetic charges, an applied magnetic field can align microscopic magnetic dipoles (e.g., spins) inside a material. The average **magnetic dipole moment per unit volume** is called **magnetization** $\vec{M}$, similar to the dielectric polarization $\vec{P}$. The **magnetic field** $\vec{B}$ in the magnetic material is a sum involving the applied magnetic field strength $\vec{H}$ and the magnetization $\vec{M}$

$$\vec{B} \;=\; \mu_0 \vec{H} + \vec{M}. \tag{10.1}$$

When comparing the definition of the magnetization (10.1) with the definition of the dielectric displacement (9.1), we note a symmetry in the units, which motivates this convention (which is a bit unusual compared to the literature).

In the absence of ferromagnetic effects (where a non-zero magnetization exists for a vanishing magnetic field strength) and for small magnetic field strengths, the magnetization is proportional to the magnetic field strength, leading to the definition of the **magnetic susceptibility** χ_m

$$\vec{M} \;=\; \mu_0 \chi_m \vec{H}. \tag{10.2}$$

In the ferromagnetic case, this can be generalized as

$$\vec{M} \;=\; \vec{M}_r + \mu_0 \chi_m \vec{H}. \tag{10.3}$$

where $\vec{M}_r$ is the remanent (ferromagnetic) magnetization (also called **remanence**) at a vanishing magnetic field $\vec{H}$.

The **magnetic permeability** μ is defined by

$$\mu \;=\; 1 + \chi_m. \tag{10.4}$$

Finally, we get an expression of $\vec{B}$ as a function of $\vec{H}$ involving the magnetic permeability

$$\vec{B} \;=\; \mu_0 \vec{H} + \vec{M} \;=\; \vec{M}_r + \mu \mu_0 \vec{H}, \tag{10.5}$$

which is symmetric to the expressions for the dielectric constant. If we also consider that (through a different magneto-optical effect) the magnetization can be created by an electric field, then more general expression reads (Schubert 2005)

$$\vec{B} \;=\; \mu_0 \vec{H} + \vec{M} \;=\; \vec{M}_r + \mu_0 \mu \vec{H} + \mu_0 \gamma \vec{E}, \tag{10.6}$$

Just like in the electrostatic case, the magnetic susceptibility χ_m and the magnetic permeability μ are 3×3-tensors, since the magnetization may not be parallel to the applied magnetic field strength vector $\vec{H}$. Therefore, $\vec{B}$ and $\vec{H}$ may not be parallel.

Also, it is very difficult for the magnetization to follow the applied field at optical frequencies. Therefore, $\mu(\omega)$ and $\gamma(\omega)$ are always zero at optical frequencies (from the infrared to the UV), but static electric

and magnetic fields can, of course, produce a magnetization, which implies that $\mu(0)$ and $\gamma(0)$ may be non-zero. Similarly to the case of the ferroelectric polarization, we may assume without loss of generality that

$$\frac{\partial \vec{M}_r}{\partial t} = 0. \tag{10.7}$$

The spatial derivatives of $\vec{M}_r$ will vanish within a single ferromagnetic domain, but they will be non-zero across domain boundaries.

Problems:

10.1. What are the units of $\vec{H}$, $\vec{B}$, $\vec{M}$, χ_μ, μ_0, and μ, in MKSA units?

11 Dielectric Response Function

As described above, the charges (and permanent electric dipoles) in a material will respond to the applied electric field and produce a dielectric polarization (see Fig. 1), but there will be a time delay. In the linear optical case (ignoring ferroeletric and magneto-optical effects), the resulting dielectric polarization can be written as (Yu & Cardona, 1996, 6.1)

$$\vec{P}(\vec{r}, t) = \epsilon_0 \int \hat{\chi}_e(\vec{r}', \vec{r}, t', t) \vec{E}(\vec{r}', t') \, dt' d^3\vec{r}', \tag{11.1}$$

where the integral is a four-dimensional infinite integral (time and space as four coordinates t' and $\vec{r}'$). If the susceptibility tensor $\hat{\chi}_e$ is a δ-function in the differences of the time and space coordinates, we recover the static expression (9.2).

Let's examine this integral (11.1): The dielectric polarization $\vec{P}(\vec{r}, t)$ depends not only on the electric field $\vec{E}(\vec{r}, t)$ applied at time t, but also on the electric fields $\vec{E}(\vec{r}, t')$ applied previously ($t' < t$). This is known as **temporal dispersion** (or simply dispersion) or **temporal non-locality**. Why is that? Because of the inertia of the charges and the related damping, it will take some time for them to respond to the applied electric field. One example is the charging of a capacitor: Because of the finite (non-zero) resistance of the wiring, the capacitor is not charged instantly, but the charge increases gradually over time and it takes an infinite amount of time for the capacitor to reach its full charge. Another example is the Lorentz model (see problems).

Similarly, a charge located at position $\vec{r}$ is influenced not only by the electric field at position $\vec{r}$, but also at positions $\vec{r}'$. Why is that? Imagine that the applied electric field is non-zero at position $\vec{r}'$ and zero everywhere else. The charge at position $\vec{r}'$ will move in response to the applied electric field by an amount $\Delta \vec{r}'$. If the distance between the charges is comparable to the magnitude of $\Delta \vec{r}'$, then nearby charges will be affected by this displacement $\Delta \vec{r}'$ and respond with their own displacement. (You can think of Fermi's exclusion principle, which does not allow two identical charges to be at the same place at the same time. You can also think of a system of coupled pendulums, where one mass is displaced and thus causes a displacement of the other masses also.) This phenomenon is called **screening**. Its effect on the dielectric susceptibility χ_e is known as **spatial dispersion** or **spatial non-locality** (sometimes just non-locality).

We conclude that the dielectric response of a material to an applied electric field is non-local in both space and time coordinates. Spatial dispersion is difficult to observe in bulk materials, but it has been found near the band-gap of semiconductors by resonant Raman scattering (Yu 1971) and even has implications for deep-UV lithography in deep-submicron CMOS lithography (Serebryakov 2003). Temporal dispersion is easily found in all materials, where the complex dielectric function usually varies with frequency.

It is impossible for the charges to respond to an electric field that has not yet been applied. This is known as **causality**. There is no mechanism in physics to predict the future (clairvoyance). Therefore,

$$\hat{\chi}_e(\vec{r}', \vec{r}, t', t) = 0 \quad \text{for} \quad t' > t. \tag{11.2}$$

15

There is no causality rule for the spatial coordinates. A charge will usually respond to an electric field applied to its right the same way as to a field applied to its left. (If the material has inversion symmetry, the two responses will be identical. If not, there may be a small difference.)

Since space and time are homogeneous (assuming an infinite homogeneous crystal, which is true if the wavelength of the electromagnetic wave is large compared to the relevant atomic length scales of the material), we can show (see problems) that (Yu & Cardona 1996, 6.2)

$$\hat{\chi}_e \left(\vec{r}', \vec{r}, t', t \right) = \chi_e \left(\vec{r}' - \vec{r}, t' - t \right). \tag{11.3}$$

Causality implies that

$$\chi_e \left(\vec{\rho}, \tau \right) = 0 \quad \text{for} \quad \tau > 0. \tag{11.4}$$

This simplifies the integral (11.1) to

$$\vec{P} \left(\vec{r}, t \right) = \epsilon_0 \int \chi_e \left(\vec{r}' - \vec{r}, t' - t \right) \vec{E} \left(\vec{r}', t' \right) dt' d^3 \vec{r}'. \tag{11.5}$$

Obviously, this is a four-dimensional convolution in time and space coordinates. Remembering the convolution theorem (3.6), we take the Fourier transform of Eq. (11.5) and obtain

$$\vec{P} \left(\vec{k}, \omega \right) = (2\pi)^2 \epsilon_0 \chi_e \left(\vec{k}, \omega \right) \vec{E} \left(\vec{k}, \omega \right). \tag{11.6}$$

The factor $4\pi^2$ is nasty and there's got to be a way to get rid of it with a different definition of the Fourier transform, but I don't know how. Who can help? Let's assume the prefactor is not there and write in a different set of units:

$$\vec{P} \left(\vec{k}, \omega \right) = \epsilon_0 \chi_e \left(\vec{k}, \omega \right) \vec{E} \left(\vec{k}, \omega \right). \tag{11.7}$$

Similarly, we can use the definition of the dielectric displacement and the dielectric function to obtain

$$\vec{D} \left(\vec{k}, \omega \right) = \epsilon_0 \epsilon \left(\vec{k}, \omega \right) \vec{E} \left(\vec{k}, \omega \right). \tag{11.8}$$

The inverse relationship

$$\vec{E} \left(\vec{k}, \omega \right) = \frac{1}{\epsilon_0} \eta \left(\vec{k}, \omega \right) \vec{D} \left(\vec{k}, \omega \right). \tag{11.9}$$

defines the loss function η, which is the inverse matrix of ϵ. (Let's keep in mind that the dielectric susceptibility χ_e and the dielectric function ϵ and its inverse η are 3×3-tensors with complex coefficients.)

A similar response function to (11.1) can be introduced to describe the response of the magnetization $\vec{M}$ to an applied magnetic field strength $\vec{H}$. Quite naturally, we find similar constitute relations

$$\vec{M} \left(\vec{k}, \omega \right) = \mu_0 \chi_m \left(\vec{k}, \omega \right) \vec{H} \left(\vec{k}, \omega \right) \quad \text{and} \tag{11.10}$$

$$\vec{B} \left(\vec{k}, \omega \right) = \mu_0 \mu \left(\vec{k}, \omega \right) \vec{H} \left(\vec{k}, \omega \right). \tag{11.11}$$

Since the magnetic response is usually very slow, we almost always have $\mu \left(\vec{k}, \omega \right) = 1$ for $\omega \neq 0$.

If we also allow magneto-electric coupling, we obtain the following constitutive relations for $\omega \neq 1$ (where ferroelectric and ferromagnetic effects can be ignored):

$$\vec{D} \left(\vec{k}, \omega \right) = \epsilon_0 \epsilon \left(\vec{k}, \omega \right) \vec{E} \left(\vec{k}, \omega \right) + \epsilon_0 \delta \left(\vec{k}, \omega \right) \vec{H} \left(\vec{k}, \omega \right) \quad \text{and} \tag{11.12}$$

$$\vec{B} \left(\vec{k}, \omega \right) = \mu_0 \mu \left(\vec{k}, \omega \right) \vec{H} \left(\vec{k}, \omega \right) + \mu_0 \gamma \left(\vec{k}, \omega \right) \vec{E} \left(\vec{k}, \omega \right). \tag{11.13}$$

Problems:

11.1. For an infinite homogeneous crystal, we are free to choose the origin of our four-dimensional space and time coordinates $\vec{r}'$ and t' in the integral (11.1) without changing the functional form of the polarization $\vec{P}(\vec{r}, t)$. Show that this implies

$$\hat{\chi}_e\left(\vec{r}', \vec{r}, t', t\right) \;=\; \chi_e\left(\vec{r}' - \vec{r}, t' - t\right).\tag{11.14}$$

11.2. Ignoring spatial dispersion, what is the dielectric response function $\epsilon\left(\vec{r}' - \vec{r}, t' - t\right)$ within the Lorentz model? (Caution: I am not sure how to solve this, but I would start with Eq. (16.15) and take the inverse Fourier transform. The resulting integral may be hard. You can solve it numerically, if you like, with the assumption $\gamma/\omega_P = 0.1$)

12 Maxwell's Equations for Homogenous Continuous Media

With these conventions for the macroscopic electric and magnetic fields, Maxwell's equations take the following differential form:

$$\text{Gauss' law (electric field)} \quad \vec{\nabla} \cdot \vec{D} = \quad \rho = 0 \tag{12.1}$$

$$\text{Gauss' law (magnetic field)} \quad \vec{\nabla} \cdot \vec{B} = \quad 0 \tag{12.2}$$

$$\text{Faraday's law} \quad \vec{\nabla} \times \vec{E} = \quad -\frac{\partial \vec{B}}{\partial t} \tag{12.3}$$

$$\text{Ampere's law} \quad \vec{\nabla} \times \vec{H} = \quad \vec{j} + \frac{\partial \vec{D}}{\partial t} = \frac{\partial \vec{D}}{\partial t}, \tag{12.4}$$

In an uncharged material without external currents, the inhomogeneous sources (charge density ρ and current density $\vec{j}$) vanish as usual.

We proceed by deriving the wave equations from Faraday's Law and Ampere's Law for the specific case of linear optics (with the possible presence of ferroeletric and ferromagnetic properties, but ruling out nonlinear effects). First, we take the curl on both sides in Faraday's Law and assume that the zero-field magnetization $\vec{M}_r$ is either homgeneous (with zero curl) or does not depend on time:

$$\vec{\nabla} \times \vec{\nabla} \times \vec{E} \;=\; \vec{\nabla} \times \left(-\frac{\partial}{\partial t}\vec{B}\right) \;=\; -\frac{\partial}{\partial t}\vec{\nabla} \times \left(\vec{M}_r + \mu\mu_0\vec{H}\right) \;=\; -\mu_0\frac{\partial}{\partial t}\vec{\nabla} \times \mu\vec{H} \tag{12.5}$$

In the isotropic case (if μ is a number, not a tensor), we could apply Ampere's Law, but not in the anisotropic case. Similarly, to evaluate $\vec{\nabla} \times \vec{\nabla} \times \vec{E} = \vec{\nabla}\left(\vec{\nabla} \cdot \vec{E}\right) - \Delta\vec{E}$, we would use Gauss' Law in the isotropic case. Unfortunately, in the anisotropic case, where $\vec{D} = \vec{P}_r + \epsilon_0\epsilon\vec{E}$, Gauss' Law only states that

$$0 \;=\; \vec{\nabla} \cdot \vec{D} = \vec{\nabla} \cdot \left(\vec{P}_r + \epsilon\epsilon_0\vec{E}\right) \;=\; \epsilon_0\vec{\nabla} \cdot \epsilon\vec{E} \tag{12.6}$$

which tells us nothing about $\vec{\nabla} \cdot \vec{E}$. (We have assumed that the remanent ferroelectric polarization is homogeneous and therefore its divergence vanishes.)

The **anisotropic wave equation** therefore reads

$$\Delta\vec{E} - \vec{\nabla}\left(\vec{\nabla} \cdot \vec{E}\right) \;=\; \mu_0\frac{\partial}{\partial t}\vec{\nabla} \times \mu\vec{H} \tag{12.7}$$

Of course, this is not really a wave equation, because we are unable to apply Ampere's Law.

A similar wave equation can be found for the magnetic field. We again assume that the remanent polarization $\vec{P}_r$ is either homogeneous or not a function of time. Taking the curl on both sides in Ampere's Law yields

$$\vec{\nabla} \times \vec{\nabla} \times \vec{H} \;=\; \vec{\nabla} \times \frac{\partial \vec{D}}{\partial t} \;=\; \frac{\partial}{\partial t}\vec{\nabla} \times \vec{D} \;=\; \epsilon_0\frac{\partial}{\partial t}\vec{\nabla} \times \epsilon\vec{E}, \tag{12.8}$$

where we are unable to apply Faraday's Law. The wave equation is

$$\Delta \vec{H} - \vec{\nabla}\left(\vec{\nabla} \cdot \vec{H}\right) \;\; = \;\; -\,\epsilon_0 \frac{\partial}{\partial t} \vec{\nabla} \times \epsilon \vec{E}. \tag{12.9}$$

Instead of two uncoupled second-order wave equations, we now have two coupled first-order equations, which we cannot simplify because of the anistropy.

In the **isotropic case**, where ϵ and μ are simple numbers (diagonal tensors with all elements equal to each other), the divergences of the fields vanish and the curl commutes with ϵ and μ. We then recover the usual **isotropic wave equations**

$$\Delta \vec{E} \;\; = \;\; \frac{\mu\epsilon}{c^2} \frac{\partial^2}{\partial t^2} \vec{E} \tag{12.10}$$

$$\Delta \vec{H} \;\; = \;\; \frac{\mu\epsilon}{c^2} \frac{\partial^2}{\partial t^2} \vec{H} \tag{12.11}$$

The phase velocity of this wave is

$$v_{\text{phase}} \;\; = \;\; \frac{c}{\sqrt{\mu\epsilon}} \tag{12.12}$$

and therefore we identify $n = \sqrt{\mu\epsilon}$ as the refractive index. In most cases (unless we deal with very exotic materials like metamaterials or photonic band gaps), μ will be equal to 1 at optical frequencies. If ϵ is less than one (for example in the x-ray regime at very high frequencies), the phase velocity will exceed the speed of light. That is not a conflict with the special theory of relativity, as long as the phase velocity remains below the speed of light.

In the more general, magneto-electric case, allowing also ferromagnetism and ferroelectricity, we have

$$\vec{\nabla} \times \vec{\nabla} \times \vec{E} \;\; = \;\; \vec{\nabla} \times \left(-\frac{\partial}{\partial t}\vec{B}\right) \;\; = \;\; -\frac{\partial}{\partial t}\vec{\nabla} \times \left(\vec{M_r} + \mu_0\mu\vec{H} + \mu_0\gamma\vec{E}\right) \quad \text{or}$$

$$\Delta \vec{E} - \vec{\nabla}\left(\vec{\nabla} \cdot \vec{E}\right) \;\; = \;\; \mu_0 \frac{\partial}{\partial t}\vec{\nabla} \times \mu\vec{H} + \mu_0 \frac{\partial}{\partial t}\vec{\nabla} \times \gamma\vec{E} \quad \text{and} \tag{12.13}$$

$$\vec{\nabla} \times \vec{\nabla} \times \vec{H} \;\; = \;\; \vec{\nabla} \times \frac{\partial \vec{D}}{\partial t} \;\; = \;\; \frac{\partial}{\partial t}\vec{\nabla} \times \left(\vec{P_r} + \epsilon_0\epsilon\vec{E} + \epsilon_0\delta\vec{H}\right) \quad \text{or}$$

$$\Delta \vec{H} - \vec{\nabla}\left(\vec{\nabla} \cdot \vec{H}\right) \;\; = \;\; -\epsilon_0 \frac{\partial}{\partial t}\vec{\nabla} \times \epsilon\vec{E} - \epsilon_0 \frac{\partial}{\partial t}\vec{\nabla} \times \delta\vec{H}, \tag{12.14}$$

since the time derivative of the ferro-electric and ferro-magnetic terms vanishes.

Instead of considering two coupled equations for $\vec{E}$ and $\vec{H}$, each with three components, it is convenient to combine both fields into a single vector with six components and a single equation.

Problems:

12.1. Simplify the anisotropic wave equations (12.13) and (12.14) for the isotropic case and vanishing magneto-electric mixing (i.e., $\delta{=}0$ and $\gamma{=}0$).

13   Generalized Plane Waves

In Snell's Law of Refraction

$$\frac{\sin\theta_1}{\sin\theta_2} = \frac{n_2}{n_1}, \tag{13.1}$$

we immediately see that there is a problem if the refractive index is complex. While we understand the meaning of a complex refractive index, where the real part describes dispersion of a wave and the imaginary part describes absorption, what is the meaning of a complex angle of refraction? To address this question, we introduce generalized plane waves.

Following Mansuripur (1995), we define a **generalized plane wave** through the same equation as previously in (6.3)

$$\vec{E}\left(\vec{r},t\right) \;=\; \vec{E}_0 \exp\left[i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right], \tag{13.2}$$

but with a complex wave vector $\vec{k}$. We might write $\vec{k}$ as

$$\vec{k} \;=\; \vec{k}_1 + i\vec{k}_2 \;=\; k_1\vec{u} + ik_2\vec{u}', \tag{13.3}$$

where $\vec{k}_1$ and $\vec{k}_2$ are ordinary vectors with real components, $\vec{u}$ and $\vec{u}'$ are unit vectors and k_1 and k_2 are real numbers. The wave (13.2) then takes the form

$$\vec{E}\left(\vec{r},t\right) \;=\; \vec{E}_0 \exp\left(-\vec{k}_2\cdot\vec{r}\right)\exp\left[i\left(\vec{k}_1\cdot\vec{r} - \omega t\right)\right]. \tag{13.4}$$

The first exponential clearly describes the attenuation of the wave according to Beer's Law, whereas the second exponential describes the oscillatory part of the wave. This generalized plane wave is similar to the solution for a damped harmonic oscillator and describes the propagation of a wave inside an attenuating (absorbing) medium.

Generalized plane waves still satisfy the relationships (6.12,6.13,6.14,6.15,6.16):

$$\vec{\nabla}\cdot\vec{E}\left(\vec{r},t\right) \;=\; i\vec{k}\cdot\vec{E} \tag{13.5}$$

$$\vec{\nabla}\times\vec{E}\left(\vec{r},t\right) \;=\; i\vec{k}\times\vec{E} \tag{13.6}$$

$$\frac{\partial\vec{E}\left(\vec{r},t\right)}{\partial t} \;=\; -i\omega\vec{E} \tag{13.7}$$

$$\vec{\nabla}^2\vec{E}\left(\vec{r},t\right) \;=\; -k^2\vec{E} \quad \text{what does this mean for complex k ???} \tag{13.8}$$

$$\frac{\partial^2\vec{E}\left(\vec{r},t\right)}{\partial t^2} \;=\; -\omega^2\vec{E} \tag{13.9}$$

$$\vec{\nabla}\left[\vec{\nabla}\cdot\vec{E}\left(\vec{r},t\right)\right] \;=\; i\vec{\nabla}\left[\vec{k}\cdot\vec{E}\right] \;=\; -\left(\vec{k}\cdot\vec{E}\right)\vec{k} \tag{13.10}$$

This definition of a generalized plan wave is not particularly interesting, if $\vec{k}_1$ and $\vec{k}_2$ are parallel, since the planes of constant phase are the same as the planes of constant amplitude. However, this statement breaks down if the two vectors are no longer parallel. In other words, the propagation of the wave might occur in a different direction than its attenuation.

14 Generalized Plane Waves in Homogenous Continuous Media

We would like to write down Maxwell's equations in $\vec{k}$-space for plane waves. The problem is, however, that plane waves with constant amplitudes $\vec{E}_0$ and $\vec{H}_0$ do not solve Maxwell's equations in an absorbing medium with absorption coefficient α, where the field strenghts decay like $\vec{E}_0\exp\left(-\alpha d/2\right)$, if d is the distance traveled in the medium. (Since the intensity decays exponentially with a penetration depth $\lambda_P = 1/\alpha$ following Beer's Law, the electric field decays with a decay constant $\alpha/2$.)

To solve Maxwell's equations for a monochromatic wave with angular frequency ω, we therefore try generalized (or inhomogeneous) plane waves

$$\vec{E}\left(\vec{r},t\right) \;=\; \vec{E}_0\exp\left[i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right] \quad \text{and} \tag{14.1}$$

$$\vec{H}\left(\vec{r},t\right) \;=\; \vec{H}_0\exp\left[i\left(\vec{k}\cdot\vec{r} - \omega t\right)\right] \tag{14.2}$$

with a complex wave vector $\vec{k} = \vec{k}_1 + i\vec{k}_2$, where the imaginary parts of the wave vector coefficients describe the exponential decay of the amplitude according to Beer's Law.

For generalized plane waves with a common complex phase factor $\exp\left[i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right]$, Maxwell's equations look as follows

$$
\begin{aligned}
\text{Gauss' law (electric field)} && \vec{k}\cdot\vec{D}_0 &= & 0 && (14.3)\\
\text{Gauss' law (magnetic field)} && \vec{k}\cdot\vec{B}_0 &= & 0 && (14.4)\\
\text{Faraday's law} && \vec{k}\times\vec{E}_0 &= & \omega\vec{B}_0 && (14.5)\\
\text{Ampere's law} && \vec{k}\times\vec{H}_0 &= & -\omega\vec{D}_0. && (14.6)
\end{aligned}
$$

Using the constitutive relations

$$
\begin{aligned}
\vec{D}_0 &= \epsilon_0\epsilon\vec{E}_0 + \epsilon_0\delta\vec{H}_0 \quad\text{and} && (14.7)\\
\vec{B}_0 &= \mu_0\mu\vec{H}_0 + \mu_0\gamma\vec{E}_0 && (14.8)
\end{aligned}
$$

similar to (9.6) and (10.6), we find the anisotropic wave equations

$$
\begin{aligned}
\left|\vec{k}\right|^2\vec{E}_0 - \left(\vec{k}\cdot\vec{E}_0\right)\vec{k} &= -\vec{k}\times\vec{k}\times\vec{E}_0 = -\omega\vec{k}\times\vec{B}_0 = -\mu_0\omega\vec{k}\times\left(\mu\vec{H}_0+\gamma\vec{E}_0\right) \quad\text{and} && (14.9)\\
\left|\vec{k}\right|^2\vec{H}_0 - \left(\vec{k}\cdot\vec{H}_0\right)\vec{k} &= -\vec{k}\times\vec{k}\times\vec{H}_0 = \omega\vec{k}\times\vec{D}_0 = \epsilon_0\omega\vec{k}\times\left(\epsilon\vec{E}_0+\delta\vec{H}_0\right) && (14.10)
\end{aligned}
$$

In the isotropic case and ignoring magneto-electric coupling, this reduces to the **isotropic wave equations**

$$
\begin{aligned}
\left|\vec{k}\right|^2\vec{E}_0 &= \mu\epsilon\frac{\omega^2}{c^2}\vec{E}_0 \quad\text{and} && (14.11)\\
\left|\vec{k}\right|^2\vec{H}_0 &= \mu\epsilon\frac{\omega^2}{c^2}\vec{H}_0. && (14.12)
\end{aligned}
$$

The dispersion relation is (CHECK use of complex variables)

$$
\left|\vec{k}\right|^2 = \mu\epsilon\frac{\omega^2}{c^2} \quad\text{or}\quad k = \sqrt{\mu\epsilon}\frac{\omega}{c}. \tag{14.13}
$$

The relationship between the electric and magnetic field strengths is now

$$
E_0 = \frac{\omega}{k}B_0 = \frac{\omega}{\sqrt{\mu\epsilon}}\frac{c}{\omega}\mu\mu_0 H_0 = \sqrt{\frac{\mu}{\epsilon}}\sqrt{\frac{\mu_0}{\epsilon_0}}H_0 = \sqrt{\frac{\mu}{\epsilon}}Z_0 H_0, \tag{14.14}
$$

where Z_0=377 Ω is the impedance of vacuum.

15   Energy Density and Energy Flow of an Electromagnetic Wave

The electromagnetic energy density (ignoring magneto-electric coupling) is (Jackson 1975)

$$
u = \frac{1}{2}\left(\vec{E}\cdot\vec{D}+\vec{H}\cdot\vec{B}\right) = \frac{1}{2}\left(\vec{E}\cdot\epsilon_0\epsilon\vec{E}+\vec{H}\cdot\mu_0\mu\vec{H}\right). \tag{15.1}
$$

In the isotropic case, we can use the impedance to eliminate the magnetic field strength to obtain

$$
u = \frac{\epsilon\epsilon_0}{2}\left|\vec{E}_0\right|^2, \tag{15.2}
$$

but this cannot be done in the anisotropic case, where the field and the response are not parallel.

In the anisotropic case, we can explicitly write Eq. (15.1) as

$$
u = \frac{1}{2}\left(E_i\epsilon_0\epsilon_{ij}E_j + H_i\mu_0\mu_{ij}H_j\right) \tag{15.3}
$$

with the usual Einstein convention for summing over repeated indices. Taking the second derivative with respect to the electric field yields (Nye 1985)

$$\frac{\partial^2 u}{\partial E_i \partial E_j} = \frac{\epsilon_0}{2} \epsilon_{ij}. \tag{15.4}$$

Since the partial derivatives commute, we find that

$$\epsilon_{ij}(\omega) = \epsilon_{ji}(\omega). \tag{15.5}$$

In other words, the dielectric tensor (and the corresponding suspectibility and conductivity tensors) are symmetric.

Poynting's theorem states that the rate of change of the energy density is related to the Poynting vector through (Jackson 1975)

$$\frac{\partial u}{\partial t} = -\vec{\nabla} \cdot \vec{S} - \vec{j} \cdot \vec{E}. \tag{15.6}$$

The second term represents the Ohmic power (product of current and voltage). For electromagnetic waves, the current $\vec{j}$ vanishes and therefore the Ohmic power is zero, leaving only the first term.

16   Dielectric Function: Drude and Lorentz Model

In Sec. 9, we discussed the response of a dielectric to a **static** electric field. How does the dielectric respond to a time-varying AC electric field? This depends on the relationship between the frequency of the field and the resonance frequency of the dielectric (let's assume there is only one). Actually, this is a damped harmonic oscillator problem. If the field varies very slowly compared to the resonance frequency of the dielectric (adiabatic case), then the charges can follow the field quite easily without a phase delay, but the amplitude will be small. As the frequency of the field increases and approaches resonance, the amplitude of the oscillation becomes very large and the phase difference between the electric field and the polarization reaches $\pi/2$. Finally, for very large frequencies of the applied electric field, the amplitude decreases again and the phase difference approaches π (see Serway 1990).

There are two very simple models called the **Lorentz** and **Drude model**, which describe the frequency-dependent dielectric functions of insulators and metals treated as a simple isotropic medium consisting of charges responding to an applied electric field (see problems). Similar models can be constructed for permanent molecular dipoles (such as in liquid water) which are randomly oriented without an electric field, but preferentially orient themselves under an applied electric field (Jackson 1975, Secs. 4.6 and 7.5(e)). In the next section, we will develop a more general framework.

In the most general case, the **Drude-Lorentz** model describes the dielectric function as

$$\epsilon(\omega) = \epsilon_\infty + \sum_i \frac{\omega_{P,i}^2}{\omega_{0,i}^2 - \omega^2 - i\gamma_i\omega} - \sum_j \frac{\omega_{P,j}^2}{\omega^2 + i\gamma_j\omega}, \tag{16.1}$$

where the first sum describes the contribution of bound carriers (with **Lorentz** terms containing the plasma frequency $\omega_{P,i}$, resonance frequency $\omega_{0,i}$ and broadening γ_i) and the second sum describes the contribution of free carriers (with **Drude** terms containing the plasma frequency $\omega_{P,j}$ and broadening γ_j).

Problems:

16.1. **Lorentz oscillator:** Derive the dielectric function $\epsilon(\omega)$ for bound charges with charge q and density n in a dielectric under the influence of an electromagnetic field $E(t) = E_0 \exp(-i\omega t)$ with a wavelength much larger than the interatomic distance. Assume that the amplitude E_0 of the electric field is small. Assume that the frictional force on the moving charge is proportional to the velocity of the charge with damping constant $b = \gamma m$. Also, assume that the restoring force on the charge is proportional to the displacement with constant k. Compare Jackson 1975, Sec. 7.5.

(a) Draw a force diagram showing all forces acting on the charge.

(b) How would you describe this type of motion in two or three words?

(c) What is the equation of motion for the charge?

(d) Determine the position of the charge as a function of time. Also, calculate the velocity and the acceleration of the charge as a function of time.

(e) What is the phase difference ϕ between the position (x) and the applied electric field $E\,(t)$ for a positive charge q.

(f) What is the magnitude of the complex susceptibility?

(g) What is the complex dielectric constant $\epsilon\,(\omega)$ as a function of angular frequency ω for this dielectric with density n of the bound charges?

(h) Calculate the static and high-frequency dielectric constants at zero and infinite frequency. What is the value of ϵ at the resonance frequency?

(i) Calculate the peak frequency and the full width at half maximum for the imaginary part of this dielectric function. What are the extrema of the real part?

(j) Plot the complex dielectric function, complex refractive index, and absorption coefficient for a Lorentz oscillator with a resonance frequency of 3 eV, scattering rate of 0.2 eV, and an oscillator strength of 3 eV.

Solution:

(a) Draw a force diagram showing all forces acting on the charge.
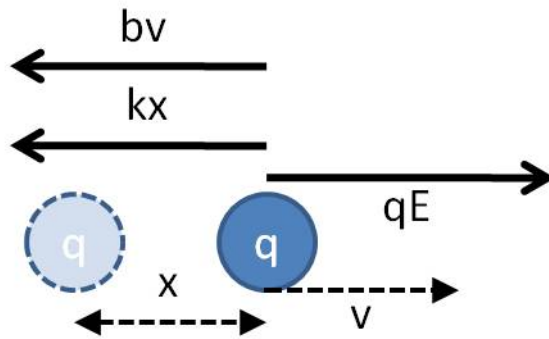
(b) How would you describe this type of motion in two or three words?
Forced oscillation (damped, harmonic).

(c) What is the equation of motion for the charge?
$F = ma$, so $qE - bv - kx = ma$.

(d) Determine the position of the charge as a function of time. Also, calculate the velocity and the acceleration of the charge as a function of time.
Substitute $x\,(t) = x_0 \exp\,(-i\omega t)$ into the equation of motion

$$qE_0 + ibx_0\omega - kx_0 \;=\; -m\omega^2 x_0 \tag{16.2}$$

$$x_0 \;=\; \frac{-qE_0}{m\omega^2 + ib\omega - k} \tag{16.3}$$

$$x\,(t) \;=\; \frac{-qE_0}{m\omega^2 + ib\omega - k}\exp\,(-i\omega t) \tag{16.4}$$

$$v\,(t) \;=\; \frac{qi\omega E_0 \exp\,(-i\omega t)}{m\omega^2 + ib\omega - k} \tag{16.5}$$

$$a\,(t) \;=\; \frac{q\omega^2 E_0 \exp\,(-i\omega t)}{m\omega^2 + ib\omega - k} \tag{16.6}$$

Let us define the **resonance frequency** ω_0 of the undamped oscillator as

$$\omega_0 \;=\; \sqrt{\frac{k}{m}} \quad \text{or} \quad k \;=\; m\omega_0^2. \tag{16.7}$$

22

This allows us to write the position of the charge differently

$$x(t) = \frac{-qE_0/m}{\omega^2 - \omega_0^2 + i\gamma\omega} \exp(-i\omega t) \tag{16.8}$$

This result seems unphysical, because the position becomes a complex quantity with a non-vanishing imaginary part. This is alright, because the applied electromagnetic field is also non-physical (has a non-vanishing imaginary part).

(e) What is the phase difference ϕ between the position $x(t)$ and the applied electric field $E(t)$ for a positive charge q.

The phase difference depends on the damping. If the damping constant b vanishes, then x_0 is real and the phase difference is zero (for $m\omega^2 < k$) or π (for $m\omega^2 > k$). In the case of non-zero damping, we can study the low-frequency and high-frequency limits: For zero frequency, the phase difference is still zero. For infinite frequency, the phase difference approaches π. To find the phase change in the general case, we must write the amplitude x_0 of the oscillation as a real and imagnary part and take the arctan of their ratio (CHECK !):

$$x_0 = \frac{-qE_0\left(m\omega^2 - k\right)}{\left(m\omega^2 - k\right)^2 + b^2\omega^2} + i\frac{qE_0 b\omega}{\left(m\omega^2 - k\right)^2 + b^2\omega^2} \tag{16.9}$$

$$\tan\phi = -\frac{b\omega}{m\omega^2 - k} = \frac{\gamma\omega}{\omega_0^2 - \omega^2}. \tag{16.10}$$

At the resonance frequency ($\omega = \omega_0$), $\tan\phi$ becomes infinite and the phase difference is therefore $\pi/2$.

(f) What is the complex dielectric constant $\epsilon(\omega)$ as a function of angular frequency ω for this dielectric with density n of the bound charges?

Hint: Remember that the polarization P is the dipole moment per unit volume.

$$P(t) = qnx(t) = \frac{-q^2 n}{m\omega^2 + ib\omega - k}E(t) = \epsilon_0\chi(\omega)E(t) \tag{16.11}$$

The dielectric susceptibility $\chi(\omega)$ therefore becomes

$$\chi(\omega) = \frac{-q^2 n}{\epsilon_0\left(m\omega^2 + ib\omega - k\right)}. \tag{16.12}$$

The dielectric function $\epsilon(\omega)$ equals

$$\epsilon(\omega) = 1 + \chi(\omega) = 1 - \frac{q^2 n}{\epsilon_0 m\left(\omega^2 + ib\omega/m - k/m\right)}. \tag{16.13}$$

We define the **plasma frequency** as

$$\omega_P^2 = \frac{nq^2}{m\epsilon_0}. \tag{16.14}$$

The dielectric function then becomes simplified:

$$\epsilon(\omega) = 1 - \frac{m\omega_P^2}{m\omega^2 + ib\omega - k} = 1 + \frac{\omega_P^2}{\omega_0^2 - \omega^2 - i\gamma\omega}. \tag{16.15}$$

Comment: The damping constant γ is usually much smaller than the resonance frequency ω_0. The imaginary part therefore is small far away from resonance. At frequencies much lower than the resonance frequency ($\omega \ll \omega_0$), the real part ϵ_1 is positive and increases with increasing frequency. This is known as **normal dispersion**. At very high frequencies ($\omega \gg \omega_0$), the

susceptibility (second term) is negative, but still increases with increasing frequency (normal dispersion). Because of the continuity of ϵ_1, there must be a frequency range in the vicinity of the resonance frequency, where ϵ_1 decreases from positive to negative values. This is known as **anomalous dispersion**. In these regions, the real part in the denominator is small and the imaginary part dominates, leading to a large imaginary part ϵ_2 in the region of anomalous dispersion. Compare Jackson 1975, Fig. 7.8.

(g) What is the magnitude of the complex susceptibility?

The magnitude of the susceptibility $\chi = \epsilon - 1$ is defined by $|\chi(\omega)|^2 = [\chi_1(\omega)]^2 + [\chi_2(\omega)]^2$. Using the definition of the plasma frequency (16.14), we find

$$|\chi(\omega)|^2 = \frac{1}{\left[\left(\omega^2 - \omega_0^2\right)^2 + \gamma^2\omega^2\right]^2}\left[\omega_P^4\left(\omega^2 - \omega_0^2\right)^2 + \omega_P^4\gamma^2\omega^2\right] = \frac{\omega_P^4}{\left(\omega^2 - \omega_0^2\right)^2 + \gamma^2\omega^2}. \quad (16.16)$$

By taking the square root, we obtain the answer

$$|\chi(\omega)| = \frac{\omega_P^2}{\sqrt{\left(\omega^2 - \omega_0^2\right)^2 + \gamma^2\omega^2}}. \quad (16.17)$$

(h) Calculate the static and high-frequency dielectric constants at zero and infinite frequency. What is the value of ϵ at the resonance frequency?

At zero frequency,

$$\epsilon_0 = \epsilon(\omega = 0) = 1 + \frac{\omega_P^2}{\omega_0^2}. \quad (16.18)$$

Note the definition of ϵ_0, which can easily be confused with the permittivity of the vacuum. This expression holds quite well to describe the refractive index of insulators in the near-infrared. In the high-frequency limit, we have

$$\epsilon_\infty = \epsilon(\omega \to \infty) = 1 - \frac{\omega_P^2}{\omega^2} \approx 1. \quad (16.19)$$

The high-frequency dielectric constant is just below one, which is important for x-ray optics. It is very important to remember that $\epsilon_0 > \epsilon_\infty$, because the charges can follow the low frequencies more easily than the high frequencies. At the resonance frequency, we have

$$\epsilon(\omega = \omega_0) = 1 + i\frac{\omega_P^2}{\gamma\omega_0}. \quad (16.20)$$

The real part of the susceptibility vanishes at resonance, but is the imaginary part peaked here?

(i) Calculate the peak frequency and the full width at half maximum for the imaginary part of this dielectric function. What are the extrema of the real part?

We need to write the real and imaginary parts of the dielectric function separately. We find that (16.15) becomes

$$\epsilon(\omega) = 1 - \frac{\omega_P^2\left(\omega^2 - \omega_0^2\right)}{\left(\omega^2 - \omega_0^2\right)^2 + \gamma^2\omega^2} + i\frac{\omega_P^2\gamma\omega}{\left(\omega^2 - \omega_0^2\right)^2 + \gamma^2\omega^2} = \epsilon_1 + i\epsilon_2. \quad (16.21)$$

At the peak frequency, the derivative of the imaginary part of the dielectric function vanishes. Using the **quotient rule** for derivatives

$$\left(\frac{u}{v}\right)' = \frac{uv' - u'v}{v^2}, \quad (16.22)$$

24

it is clear that the derivative of the quotient u/v will vanish, if the nominator $uv' - u'v$ vanishes Therefore, with the substitutions

$$u = \omega \qquad v = \left(\omega^2 - \omega_0^2\right)^2 + \gamma^2\omega^2 \quad \text{and} \tag{16.23}$$

$$u' = 1 \qquad v' = 4\omega\left(\omega^2 - \omega_0^2\right) + 2\gamma^2\omega, \tag{16.24}$$

we find

$$0 \; = \; 4\omega^2\left(\omega^2 - \omega_0^2\right) + 2\gamma^2\omega^2 - \left(\omega^2 - \omega_0^2\right)^2 - \gamma^2\omega^2 \; = \; 3\omega^4 - 2\omega^2\omega_0^2 - \omega_0^4 + \gamma^2\omega^2. \tag{16.25}$$

This biquadratic equation has the solution

$$\omega^2 \; = \; \frac{1}{6}\left[2\omega_0^2 - \gamma^2 \pm \sqrt{(2\omega_0^2 - \gamma^2)^2 + 12\omega_0^4}\right]. \tag{16.26}$$

or

$$6\omega^2 \; = \; 2\omega_0^2 - \gamma^2 \pm \sqrt{(2\omega_0^2 - \gamma^2)^2 + 12\omega_0^4} \; = \; 2\omega_0^2 - \gamma^2 \pm \sqrt{16\omega_0^4 - 4\omega_0^2\gamma^2 + \gamma^4}. \tag{16.27}$$

Since the term under the square root is not a complete square, we can only simplify this expression in the limit $\gamma \ll \omega_0$ and find the approximate position of the peak in the imaginary part of the susceptibility to lowest order in γ. It is obvious that we need the solution with the plus sign to obtain a positive value of ω^2.

$$6\omega^2 \; = \; 2\omega_0^2 - \gamma^2 \pm 4\omega_0^2\sqrt{1 - \frac{\gamma^2}{4\omega_0^2}} \; \approx \; 2\omega_0^2 - \gamma^2 + 4\omega_0^2\left(1 - \frac{\gamma^2}{8\omega_0^2}\right) \; = \; 6\omega_0^2 - \frac{3}{2}\gamma^2 \tag{16.28}$$

By taking the square root and again keeping terms to first order in γ/ω_0, we find

$$\omega_{\text{peak}} \; = \; \sqrt{\omega_0^2 - \gamma^2/4} \; \approx \; \omega_0\left(1 - \frac{\gamma^2}{8\omega_0^2}\right). \tag{16.29}$$

As expected, the damping shifts the peak to lower energies. For $\omega_0 = 3$ eV and $\gamma = 0.2$ eV, this shift equals 0.5 meV. The shift grows to 0.037 eV, if we keep $\omega_0 = 3$ eV, but increase γ to 1 eV. Since this shift is much smaller than the full width at half maximum of the peak, it will be difficult to see experimentally.

To find the peak amplitude of the imaginary part of the dielectric function, we insert our solution (16.29) into the Lorentz oscillator equation (16.21). Thus we find

$$\epsilon_2\left(\omega_{\text{peak}}\right) \; = \; \frac{\omega_P^2}{\gamma\omega_0}\left(1 + \frac{\gamma^2}{16\omega_0^2}\right). \tag{16.30}$$

For typical values of $\omega_0 = 3$ eV and $\gamma = 0.1$ eV, the correction to the peak amplitude given in (16.20) is about 7×10^{-5} and therefore negligible.

To show that the full width at half maxium is γ, we must use (16.21) to evaluate

$$\epsilon_2\left(\omega_{\text{peak}} - \gamma/2\right) \; \approx \; \epsilon_2\left(\omega_0 - \gamma/2\right) \; = \tag{16.31}$$

and

$$\epsilon_2\left(\omega_{\text{peak}} + \gamma/2\right) \; \approx \; \epsilon_2\left(\omega_0 + \gamma/2\right) \; = \tag{16.32}$$

to first order in γ, ignoring terms on the order of γ^2.

(j) Plot the complex dielectric function, complex refractive index, and absorption coefficient for a Lorentz oscillator with a resonance frequency of 3 eV, scattering rate of 0.2 eV, and a plasma frequency of 3 eV.
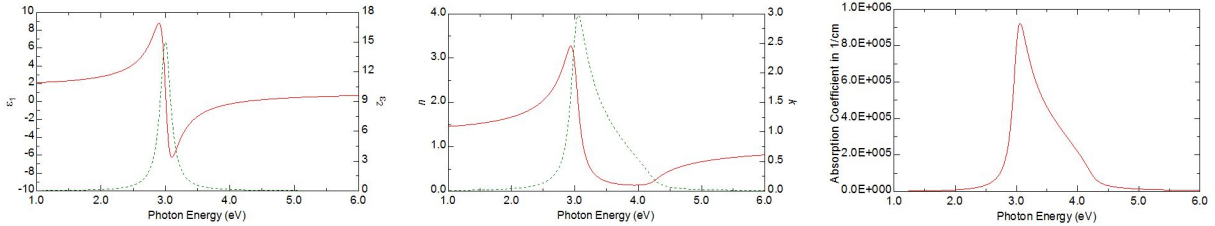
A few items are worth noting: (1) Since the plasma frequency and the resonance frequency are equal, the low-frequency limit of the dielectric constant is 1+1=2. (2) The imaginary part ϵ_2 is very symmetric and peaks at the resonance frequency. The real part ϵ_1 has a resonance-type lineshape and also looks pretty symmetric around the resonance frequency. (3) The refractive index and the extinction coefficient are very asymmetric. (4) The real part ϵ_1 crosses one right at the resonance frequency (and later becomes negative). (5) The absorption oefficient and the extinction coefficient are related by $\alpha = \frac{4\pi}{\lambda}k$. If the broadening is much smaller than the peak energy, the prefactor is nearly constant around the peak. Therefore, the shape of the peaks of α and κ are very similar. Both have peaks near 3.06 eV, shifted to higher energies compared to the peak of ϵ_2 at 3 eV.

16.2. A Lorentz oscillator with zero broadening (damping) is called a **pole**. What is the dielectric function for a pole? Write the expression for the pole as a function of wavelength and compare it with the **Cauchy** and **Sellmeier** expressions.

Solution: The imaginary part of ϵ is proportional to the damping b or γ and therefore vanishes. The dielectric function is real and has a pole (diverges) at $\omega = \omega_0$:

$$\epsilon(\omega) = 1 + \frac{\omega_P^2}{\omega_0^2 - \omega^2} \tag{16.33}$$

As a function of wavelength λ, this becomes

$$\epsilon(\lambda) = 1 + \frac{\omega_P^2}{\omega_0^2 - (2\pi c/\lambda)^2} = 1 + \frac{\omega_P^2 \lambda^2}{\omega_0^2 \lambda^2 - 4\pi^2 c^2} = 1 + \frac{B\lambda^2}{\lambda^2 - C} \tag{16.34}$$

with adjustable coefficients B and C, which is known as the **Sellmeier equation** for $\epsilon_1 = n^2$ in transparent glasses (Wikipedia). To get a good description for glass, one actually needs to add several terms with this function form (i.e., several Sellmeier expressions are needed). We conclude that the Sellmeier expression is an expansion in several Lorentz oscillators with zero damping.

Comments: In practice, the refractive index (or the dielectric function) of an insulator in its transparent region is often described by two poles, one above and one below the transparent spectral range. From a materials physics perspective, we can think of the infrared pole (below the transparent spectral range) as a phonon reststrahlen band (lattice vibrations), which are usually in the 10 to 100 meV range. Similarly, the pole above the transparent region describes the onset of absorption (band gap) of the material, usually in the UV between 3 and 10 eV. For BK7 borosilicate crown glass, Wikipedia lists the two poles in the UV at 77 and 141 nm plus one in the infrared near 10 μm. The **Cauchy equation**

$$n(\lambda) = \sqrt{\epsilon(\lambda)} = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} \tag{16.35}$$

is different, but it can be viewed as a Laurent expansion of the Sellmeier equation

$$n(\lambda) = \sqrt{\epsilon(\lambda)} = \sqrt{1 + \frac{B\lambda^2}{\lambda^2 - C}}. \tag{16.36}$$

16.3. Model the refractive index and the dielectric function of BK7 glass, sapphire (ordinary and extraordinary direction), and fused silica (quartz) from 190 to 2500 nm (0.5 to 6.6 eV) using the Sellmeier coefficients found in Wikipedia. Plot the results in units of wavelength and of photon energy. First use a spreadsheet program like Excel, then use the the Woollam software to achieve the same plots. Copy and paste your figures into a Word document.

16.4. **Drude model for the optical response of metals:** In a metal, the charges are free to move around. Thus the restoring force vanishes ($k=0$, $\omega_0=0$).

(a) What is the dielectric function within the Drude model? Separate the real and imaginary terms.
(b) If we neglect damping, what happens at the plasma frequency ω_P?
(c) What is the dielectric function of a metal at high frequencies ($\omega \gg \gamma$)?
(d) Plot the real and imaginary parts of the dielectric function in units of $x = \omega/\omega_P$ from 0.2 to 2. Assume that $\gamma = 0.1\omega_P$.

Solution:

(a) What is the dielectric function within the Drude model? Separate the real and imaginary terms. From Eq. (16.15), we obtain (Jackson, 1975, 7.56)

$$\epsilon(\omega) = 1 - \frac{m\omega_P^2}{m\omega^2 + ib\omega} = 1 - \frac{\omega_P^2}{\omega^2 + i\gamma\omega} = 1 + i\frac{\omega_P^2}{\omega(\gamma - i\omega)}. \qquad (16.37)$$

In components, this reads

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + \gamma^2} + i\frac{\omega_P^2}{\omega^2 + \gamma^2} \times \frac{\gamma}{\omega}. \qquad (16.38)$$

The plasma frequency $\omega_P^2 = nq^2/m\epsilon_0$ depends on the charge density n of the metal and the mass m of the carriers. (Sometimes an **effective mass** is used to describe the motion of the carriers in the metal, which is different from the mass of the same charge in vacuum.) The **scattering rate** γ describes the friction of carriers in the metal. We see that the imaginary part of smaller than the real part by a factor γ/ω.

(b) If we neglect damping, what happens at the plasma frequency ω_P?
The dielectric constant ϵ_1 vanishes at the plasma frequency ω_P, if we neglect damping.

(c) What is the dielectric function of a metal at high frequencies ($\omega \gg \gamma$)?
In this approximation, we have (Jackson 1975, Sec. 7.5 (d))

$$\epsilon(\omega) \approx 1 - \frac{\omega_P^2}{\omega^2}. \qquad (16.39)$$

If the angular frequency is below the plasma frequency (but still much larger than the damping), then the dielectric constant is negative. The light penetrates only a very short distance into the metal and is almost entirely reflected (**this needs to be shown later**). For frequencies above the plasma frequency, the dielectric function is now real and positive and the metal becomes transparent. This can actually be observed in the UV region for many metals.

(d) Plot the real and imaginary parts of the dielectric function in units of $x = \omega/\omega_P$ from 0.2 to 2. Assume that $\gamma = 0.1\omega_P$.
In units of $x = \omega/\omega_P$, we need to plot

$$\epsilon_1(x) = 1 - \frac{1}{x^2 + 0.01} \qquad (16.40)$$

$$\epsilon_2(x) = \frac{1}{x^2 + 0.01} \times 0.1 \qquad (16.41)$$

There are number of interesting things to note in this plot: First, the real part diverges towards $-\infty$, while the imaginary part diverges towards $+\infty$. No DC electric field can exist in a metal,

therefore the absorption becomes infinitely large at small frequencies. Second, the imaginary part is much smaller than the real part (by a factor of γ/ω). Finally, the real part crosses zero approximately at the plasma frequency.
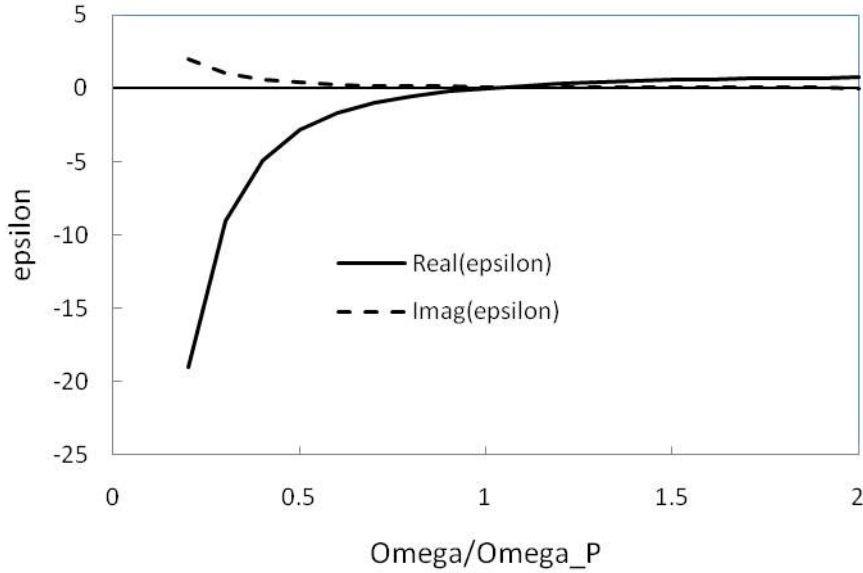
(e) To avoid the Drude divergence of $\epsilon(\omega)$ for low frequencies, one defines the complex optical conductivity as

$$\sigma(\omega) = -i\epsilon_0\omega\left[\epsilon(\omega) - 1\right]. \tag{16.42}$$

Show that the Drude contribution to the optical conductivity equals

$$\sigma(\omega) = \frac{\epsilon_0\omega_P^2}{\omega^2 + \gamma^2}(\gamma + i\omega) = \frac{\epsilon_0\omega_P}{(\omega/\omega_P)^2 + (\gamma/\omega_P)^2}(\gamma/\omega_P + i\omega/\omega_P) \tag{16.43}$$

Draw a figure showing the real and imaginary part of σ as a function of frequency. Assume $\gamma/\omega_P = 0.1$ and define $x = \omega/\omega_P$. Draw the figure from $x=0$ to $x=2$.

17 Macroscopic Optical Constants

Complex refractive index n
    Refrative index N
    Extinction coefficient k.
    Reflected intensity equals

$$R = \left|\frac{n-1}{n+1}\right|^2 = \left|\frac{N+ik-1}{N+ik+1}\right|^2 \tag{17.1}$$

Complex optical conductivity
Calculate reflected intensity for the Lorentz and Drude model and discuss.

Problems:

17.1. Consider a Drude metal with a plasma frequency of 10 eV and a broadening of 1 eV. Prepare publication-quality figures with figure captions showing the following quantities (a) complex dielectric function; (b) complex refractive index (refractive index N and extinction coefficient k); (c) reflection coefficient; (d) absorption coefficient (in units of cm^{-1}); (e) complex optical conductivity σ. Choose a suitable range of photon energies in your plots to show all the important physics. Use complete sentences to describe the features shown in the figures in relationship to the parameters of the Drude oscillator model. Do not use color unless required to increase the information content of the figure.

17.2. Consider an insulator with the following parameters to describe lattice vibrations: Amplitude $A=3$, TO energy 10 meV, broadening 1 meV. Prepare publication-quality figures with figure captions showing the following quantities (a) complex dielectric function; (b) complex refractive index (refractive index N and extinction coefficient k); (c) reflection coefficient; (d) absorption coefficient (in units of cm^{-1}); (e) complex optical conductivity σ. Choose a suitable range of photon energies in your plots to show all the important physics. Use complete sentences to describe the features shown in the figures in relationship to the parameters of the Lorentz oscillator model. Do not use color unless required to increase the information content of the figure.

17.3. Calculate $\hbar c$ in units of $eVcm^{-1}$. For a Drude metal with a plasma frequency of 10 eV and a broadening parameter of $\gamma=1$ eV, calculate the absorption coefficient (in units of cm^{-1} at 2 eV.

17.4. Show analytically that within the Drude model the reflectivity R approaches 1 and the absorption coefficient α goes to zero, as the frequency goes to zero. (Hint: Use a Taylor expansion of the Drude dielectric function for small ω.

17.5. Within the Drude model, calculate the reflectance at the plasma frequency to first order in γ/ω_P, where γ is much less than ω_P.

18 Causality, Kramers-Kronig-Relations, and Sum Rules

We remember from the theory of functions with complex variables (Janich 1983) that any well-behaved complex function $f(z)$ (which is analytical everywhere in the complex plane except for a finite number of poles) can be written as a Laurent series

$$f(z) = \frac{g(z)}{h(z)} = \sum_{n=-\infty}^{\infty} a_n (z-z_0)^n, \tag{18.1}$$

where $g(z)$ and $h(z)$ are analytical functions, usually polynomials with complex coefficients. For such a function, the residual of f at z_0 defined by

$$\text{Res}_{z_0} f = \frac{1}{2\pi i} \oint_{|z-z_0|=r} f(z)\,dz \tag{18.2}$$

can be calculated as follows, if f has a pole at z_0 of no higher order than k:

$$\text{Res}_{z_0} f = \frac{1}{(k-1)!} \frac{d^{k-1}}{dz^{k-1}} (z-z_0)^k f(z) \Big|_{z=z_0} \tag{18.3}$$

If f has a simple pole ($k=1$) at z_0, then

$$\text{Res}_{z_0} f = \frac{g(z_0)}{h'(z_0)}. \tag{18.4}$$

We now remember from (11.4) that the dielectric response function $\chi_e(\tau) = 0$ for $\tau>0$, i.e., it vanishes for positive times. The complex function χ_e therefore vanishes in the upper complex half plane. We assume that it is analytical in the lower complex half plane, including the real axis.

19 Analytical properties of the dielectric function

Since the electric field $\vec{E}(\vec{r}, t)$ and the polarization $\vec{P}(\vec{r}, t)$ are real quantities, the susceptibility and the dielectric function must satisfy the condition

$$\epsilon\left(-\vec{k}, -\omega\right) = \overline{\epsilon\left(\vec{k}, \omega\right)}, \tag{19.1}$$

$$\chi\left(-\vec{k}, -\omega\right) = \overline{\chi\left(\vec{k}, \omega\right)}, \tag{19.2}$$

where $\bar{\epsilon}$ is the complex conjugate of ϵ. One can also show that

$$\epsilon\left(-\vec{k},\omega\right) = {}^{t}\epsilon\left(\vec{k},\omega\right) \quad \text{and} \quad \chi\left(-\vec{k},\omega\right) = {}^{t}\chi\left(\vec{k},\omega\right), \tag{19.3}$$

which is known as the **Onsager relation**.

Ignoring spatial dispersion, we write

$$\vec{P}\left(\omega\right) = \epsilon_0\chi_e\left(\omega\right)\vec{E}\left(\omega\right), \tag{19.4}$$

$$\vec{D}\left(\omega\right) = \epsilon_0\epsilon\left(\omega\right)\vec{E}\left(\omega\right), \tag{19.5}$$

$$\vec{E}\left(\omega\right) = \frac{1}{\epsilon_0}\eta\left(\omega\right)\vec{D}\left(\omega\right). \tag{19.6}$$

This implies

$$\epsilon\left(-\omega\right) = \overline{\epsilon\left(\omega\right)}, \tag{19.7}$$

$$\eta\left(-\omega\right) = \overline{\eta\left(\omega\right)}, \tag{19.8}$$

$$\chi\left(-\omega\right) = \overline{\chi\left(\omega\right)}, \tag{19.9}$$

$$\epsilon\left(\omega\right) = {}^{t}\epsilon\left(\omega\right) \tag{19.10}$$

$$\chi\left(\omega\right) = {}^{t}\chi\left(\omega\right) \tag{19.11}$$

$$\eta\left(\omega\right) = {}^{t}\eta\left(\omega\right). \tag{19.12}$$

The dielectric, loss function, and susceptibility tensors are therefore symmetric.

A proof for the symmetry of the tensor properties can be derived from energy considerations and is given by Nye (1985). The energy density of the wave is

$$u = \frac{1}{2}\left(\vec{E}\cdot\vec{D} + \vec{H}\cdot\vec{B}\right) = \frac{1}{2}\left(\vec{E}\cdot\epsilon_0\epsilon\vec{E} + \vec{H}\cdot\mu_0\mu\vec{H}\right) = \frac{1}{2}\left(E_i\epsilon_0\epsilon_{ij}E_j + H_i\mu_0\mu_{ij}H_j\right), \tag{19.13}$$

where the right hand side of the equation uses the Einstein convention for summing over repeated indices. Since the derivatives with respect to the fields along the i and j directions commute, we have

$$\frac{\epsilon_0}{2}\epsilon_{ij} = \frac{\partial^2 u}{\partial E_i \partial E_j} = \frac{\partial^2 u}{\partial E_j \partial E_i} = \frac{\epsilon_0}{2}\epsilon_{ji}, \tag{19.14}$$

with a similar equation for the permeability and magnetic susceptibility.

Berreman and Unterwald (1968) note that any complex analytical function can be written as a Laurent series (Jahnich 1983)

$$\epsilon\left(\omega\right) = \frac{\displaystyle\prod_{m=1}^{M}\left(\omega - Z_m\right)}{\displaystyle\prod_{n=1}^{N}\left(\omega - P_n\right)} \tag{19.15}$$

with as many zeroes Z_m and poles P_n as needed. Since $\epsilon \to 1$ for $\omega \to \infty$, the number of poles must be equal to the number of zeroes ($M = N$). The poles are near the **TO frequencies** and the zeroes are near the **LO frequencies**. See (19.25) for an exact relationship between the LO/TO energies and broadenings and the location of the zeroes and poles.

To satisfy the relations (19.1) and (19.7), the poles and zeroes must be symmetric around the imaginary axis. In other words, if P_n is a pole and Z_m a zero, then $-\overline{P}_n$ is also a pole and $-\overline{Z}_m$ is also a zero (Lowndes 1970). This reduces the dielectric function to (Lowndes 1970)

$$\epsilon\left(\omega\right) = \epsilon_\infty \prod_{j=1}^{N} \frac{\omega_{\mathrm{LO},j}^2 - \omega^2 - i\gamma_{\mathrm{LO},j}\omega}{\omega_{\mathrm{TO},j}^2 - \omega^2 - i\gamma_{\mathrm{TO},j}\omega}. \tag{19.16}$$

The quantity ϵ_∞ was introduced to account for the effects of poles and zeroes are very large frequencies (high above the experimentally observed range), whose effect is only a multiplication with a constant, without any influence on the spectral dispersion.

Because of causality, the poles and zeroes must all be below the real axis (this must be shown, Berreman & Unterwald cite Davidov, 1965, Sec. 112).

By comparing the **Lowndes** equation (19.16) with the Drude-Lorentz model (16.1), we find that we have replaced the sum of Lorentz terms with a product of similar fractions. We now allow distinct broadenings for the TO and LO vibration modes, whereas only one broadening parameter was contained in each Lorentz term. It helps to remember the key assumptions underlying the Lorentz model: (1) The response of charges to an electromagnetic field is harmonic and the restoring force is proportional to the displacement. (2) The frictional force is proportional to the velocity of the charges. (3) There is no interaction between charges of different types. The Lowndes model does not make any of these assumptions and only has the analyticity of the dielectric function as its basis. If some poles or zeroes are close to each other (relative to the damping parameter), a better fit to experimental data is often achieved with the Lowndes model. Allowing different broadening parameters for the TO and LO vibrations is equivalent to a frequency-dependent damping term in the uncoupled (Lorentz) oscillator (Berreman & Unterwald 1968).

Problems:

19.1. Show that (Yu & Cardona 1996)

$$\epsilon\left(-\vec{k}, -\omega\right) \;=\; \overline{\epsilon\left(\vec{k}, \omega\right)}, \tag{19.17}$$

where $\bar{\epsilon}$ is the complex conjugate of ϵ. Remember that the observable quantities $\vec{E}\left(\vec{r}, t\right)$ and $\vec{D}\left(\vec{r}, t\right)$ as a function of space and time coordinates must be real. Therefore, the tensor $\epsilon\left(\vec{r}, t\right)$ must have real components also.

19.2. Show that (Yu & Cardona 1996, Nye 1985)

$$\epsilon\left(-\vec{k}, \omega\right) \;=\; {}^t\epsilon\left(\vec{k}, \omega\right), \tag{19.18}$$

where ${}^t\epsilon$ is the transposed matrix of ϵ. (This is known as the **Onsager relation**.)

19.3. Lowndes (1970) claims that $\epsilon\left(\omega\right) = -\overline{\epsilon\left(\omega\right)}$, due to the causal relationship between the electric field and the dielectric displacement. Does this make sense? Also, he claims that causality requires the poles and zeroes of $\epsilon\left(\omega\right)$ to be in the negative complex plane (below the real axis). Can you show this?

19.4. If the dielectric function has the form

$$\epsilon\left(\omega\right) \;=\; \prod_{j=1}^{2N} \frac{\omega - Z_j}{\omega - P_j}, \tag{19.19}$$

with zeroes Z_j and poles P_j, show that the poles and zeroes are symmetric relative to the imaginary axis in the complex plane. What is the physical reason behind this? Use this symmetry property to write the dielectric function as a product of N terms with quadratic polynomials in the numerator and denominator. Find the relationship between the zeroes Z_j and poles P_j and the LO and TO energies and broadenings specified in (19.16).

Solution: By evaluating (19.19) for negative frequencies, we conclude that

$$\epsilon\left(-\omega\right) \;=\; \prod_{j=1}^{2N} \frac{-\omega - Z_j}{-\omega - P_j} \;=\; \prod_{j=1}^{2N} \frac{\omega + Z_j}{\omega + P_j} \;=\; \prod_{j=1}^{2N} \frac{\omega - \left(-Z_j\right)}{\omega - \left(-P_j\right)}. \tag{19.20}$$

Since the fields must be real, the property (19.7) requires that

$$\epsilon\left(-\omega\right) \;=\; \overline{\epsilon\left(\omega\right)} \;=\; \prod_{j=1}^{2N} \frac{\omega - \overline{Z_j}}{\omega - \overline{P_j}}. \tag{19.21}$$

By comparing (19.20) and (19.21) and taking the complex conjugate, we find that

$$\epsilon\left(\omega\right) \;=\; \prod_{j=1}^{2N} \frac{\omega - Z_j}{\omega - P_j} \;=\; \prod_{j=1}^{2N} \frac{\omega - \left(-\overline{Z_j}\right)}{\omega - \left(-\overline{P_j}\right)}. \tag{19.22}$$

For this to be true at any frequency, the zeroes Z_j and $-\overline{Z_j}$ must belong to the same set, which proves that the zeroes are symmetric relative to the imaginary axis. The same argument holds for the poles. The physical reason behind this relationship is the fact that the electromagnetic fields must be real quantities. We can use the symmetry property to reduce the number of products as

$$
\begin{aligned}
\epsilon\left(\omega\right) \;=\; & \prod_{j=1}^{2N} \frac{\omega - Z_j}{\omega - P_j} \;=\; \prod_{j=1}^{N} \frac{\left(\omega - Z_j\right)\left(\omega + \overline{Z_j}\right)}{\left(\omega - P_j\right)\left(\omega + \overline{P_j}\right)} \;=\; \prod_{j=1}^{N} \frac{\omega^2 + \omega\overline{Z_j} - \omega Z_j - Z_j\overline{Z_j}}{\omega^2 + \omega\overline{P_j} - \omega P_j - P_j\overline{P_j}} \;=\; \\
\;=\; & \prod_{j=1}^{N} \frac{\omega^2 - |Z_j|^2 + \omega\left(\overline{Z_j} - Z_j\right)}{\omega^2 - |P_j|^2 + \omega\left(\overline{P_j} - P_j\right)} \;=\; \prod_{j=1}^{N} \frac{|Z_j|^2 - \omega^2 + \omega\left(Z_j - \overline{Z_j}\right)}{|P_j|^2 - \omega^2 + \omega\left(P_j - \overline{P_j}\right)}.
\end{aligned} \tag{19.23}
$$

Considering that $z - \bar{z} = 2\mathrm{Im}\left(z\right)$ for any complex number z, we conclude that

$$\epsilon\left(\omega\right) \;=\; \prod_{j=1}^{N} \frac{|Z_j|^2 - \omega^2 + 2\omega\mathrm{Im}\left(Z_j\right)}{|P_j|^2 - \omega^2 + 2\omega\mathrm{Im}\left(P_j\right)}. \tag{19.24}$$

A comparison with (19.16) yields

$$\omega_{\mathrm{LO}} \;=\; |Z_j|; \quad \omega_{\mathrm{TO}} \;=\; |P_j|; \quad \gamma_{\mathrm{LO}} \;=\; -2\mathrm{Im}\left(Z_j\right); \quad \gamma_{\mathrm{TO}} \;=\; -2\mathrm{Im}\left(P_j\right); \tag{19.25}$$

20   Experimental Assignments

20.1. Turn off the Xe lamp. Insert the monochromator calibration lamp into the side port of the spacer between the Xe lamp and the monochromator. Optimize the intensity in white-light configuration of the monochromator. Acquire transmission spectra to obtain the wavelengths of the spectral lines emitted by the lamp. How does the width of these lines vary with the slit width of the monochromator? Derive an expression for the linear dispersion of the monochromator (in nm/mm). Compare with the manual.

20.2. Acquire a transmission spectrum of the Xe short-arc lamp. Interpret what you see in the spectrum, based on the absorption in the optical fiber, the spectral lines of the monochromator, the grating changes, and the filter wheel. Compare with the `hardware.cnf` file describing the configuration of the instrument.

20.3. Purchase some colored glass at a hobby store. Acquire transmission spectra for colored glass. Can you calculate the absorption coefficient (in cm^{-1}) for the material? (Schott glass filters can also be used, but they are more expensive, probably.)

20.4. Acquire isotropic ellipsometry data with depolarization for the series of AlN films on Si. Fit the data using a Cauchy layer with an Urbach tail over the transparent region of the spectrum. Next, use the GenOsc model with increasing complexity to better describe the data in the range of absorption. What is the band gap of the material?

21 References

Ashcroft & Mermin 1976 N.W. Ashcroft and N.D. Mermin, *Solid State Physics* (Saunders, Philadelphia, 1976).

Berreman & Unterwald 1968 D.W. Berreman and F.C. Unterwald, *Adjusting poles and zeros of dielectric dispersion to fit reststrahlen of $PrCl_3$ and $LaCl_3$*, Phys. Rev. **174**, 791-799 (1968).

Fox 2010 M. Fox, *Optical Properties of Solids* (Oxford University Press, Oxford, 2010).

Fujiwara 2007 H. Fujiwara, *Spectroscopic Ellipsometry: Principles and Applications* (Wiley, Chichester, 2007).

Good & Nelson 1971 R.H. Good and T.J. Nelson, *Classical Theory of Electric and Magnetic Fields* (Academic Press, New York, 1971).

Holm 1991 R.T. Holm, *Convention confusions*, in *Handbook of Optical Constants of Solids II*, edited by E.D. Palik (Academic Press, Boston, 1991), p. 21-55).

Humlíček 2005 J. Humlíček, *Polarized Light and Ellipsometry*, in *Handbook of Ellisometry*, edited by H.G. Tompkins and E.A. Irene (William Andrew, Norwich, NY, 2005), p. 3-91.

Jackson 1975 J.D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975, 2nd edition).

Lowndes 1970 R.P. Lowndes, *Influence of lattice anharmonicity on the longitudinal optic modes of cubic ionic solids*, Phys. Rev. B **1**, 2754 (1970).

Mansuripur 1995 M. Mansuripur, *The Physical Principles of Magneto-Optical Recording* (Cambridge University Press, Cambridge, 1995).

Muller 1969 R.H. Muller, *Definitions and conventions in ellipsometry*, Surf. Sci. **16**, 14-33 (1969).

Nye 1985 J.F. Nye, *Physical Properties of Crystals* (Clarendon, Oxford, 1985).

Serebryakov 2003 A.G. Serebryakov, F. Bociort, and J. Braat, *Spatial dispersion of crystals as a critical problem for deep UV lithography*, J. Opt. Technol. **70**, 566-569 (2003).

Schubert 2005 M. Schubert, *Theory and Application of Generalized Ellipsometry*, in *Handbook of Ellisometry*, edited by H.G. Tompkins and E.A. Irene (William Andrew, Norwich, NY, 2005), p. 637-717.

Serway 1990 R.A. Serway, *Physics for Scientists & Engineers* (Saunders, Philadelphia, 1990, 3rd edition).

Young & Freedman 2007 H.D. Young and R.A. Freedman, *University Physics* (Pearson, San Francisco, 2007, 12th edition).

Yu 1971 P.Y. Yu and M. Cardona, *Spatial dispersion in the dielectric constant of GaAs*, Solid State Commun. **9**, 1421 (1971).

Yu 1996 P.Y. Yu and M. Cardona, *Fundamentals of Semiconductors* (Springer, Berlin, 1996).