Chapter 3

Light propagation in dielectric materials

The time-dependent Maxwell equations are frequently used as a mathematical framework to describe the propagation of light in dielectric materials. In this chapter we closely follow [16] to describe light propagation in conventional dielectric materials. Then concepts are generalized to describe light propagation in homogeneous isotropic negative index materials and in photonic crystals.

3.1 Conventional lossless dielectric materials

3.1.1 Velocity of light and refraction index

From Maxwell’s equations (see Eq. (2.4)) it follows that if the medium is homogeneous, in addition to be isotropic, and if there are no electric and magnetic currents, the equations for the electric field vector \( E \) and the magnetic field vector \( H \) are given by

\[
\nabla^2 E - \varepsilon \mu \frac{\partial^2 E}{\partial t^2} = 0, \tag{3.1a}
\]

\[
\nabla^2 H - \varepsilon \mu \frac{\partial^2 H}{\partial t^2} = 0. \tag{3.1b}
\]

Eqs. (3.1a) and (3.1b) are standard equations of wave motion and suggest the existence of electromagnetic waves propagating with a velocity

\[
v = 1/\sqrt{\varepsilon \mu} = c/\sqrt{\varepsilon \mu r}, \tag{3.2}
\]
where $c = 1 / \sqrt{\varepsilon_0 \mu_0}$ denotes the velocity of light in vacuum ($\approx 3 \times 10^8$ m/s). Since usually $\varepsilon_r > 1$ and $\mu_r \approx 1$ for transparent substances, the velocity $v$ is smaller than the velocity of light in vacuum. The velocity $v$ is usually determined only relative to $c$ by making use of the law of refraction or Snell’s law (for a derivation see [16] and Section 3.1.5)

$$\sin \theta_1 \sin \theta_2 = \frac{v_1}{v_2} = n_{12},$$

(3.3)

where $\theta_1$ and $\theta_2$ are the angles made by the electromagnetic wave with the normal of the interface between the media 1 and 2, in the first and second medium, respectively (see Fig. 3.1) and $n_{12}$ denotes the refractive index for refraction from the first into the second medium. The absolute refractive index $n$ of a medium, that is the refractive index for refraction from vacuum into that medium is defined as

$$n = \frac{c}{v},$$

(3.4)

Hence,

$$n_{12} = \frac{n_2}{n_1} = \frac{v_1}{v_2},$$

(3.5)

where $n_1$ and $n_2$ are the absolute refractive indices of medium 1 and 2, respectively. From Eqs. (3.2) and (3.4) follows the Maxwell formula

$$n = \sqrt{\varepsilon_r \mu_r},$$

(3.6)

For non-magnetic materials $\mu_r \approx 1$. In general $\varepsilon_r$ depends on the frequency $\omega$ of the electromagnetic field. In this way the atomic structure and the dynamics of matter can be taken into...
3.1. Conventional lossless dielectric materials

For the numerical simulations presented in this and the following chapters, however, we assume that $\varepsilon_r$ does not depend on frequency. Materials with real and positive material parameters $\varepsilon_r$ and $\mu_r$ are often called conventional lossless dielectric materials.

3.1.2 Phase, group front and group velocity

The velocity of a wave is an important concept for practical applications (for example, signal transmission). For wave packets two velocities are of importance, the phase and the group velocity. The realization of materials showing negative refraction of light created a dispute about the sign of the phase and group velocity [53–55]. Much of the confusion was caused by inconsistent definitions of the group velocity. A clear formulation of wave propagation, with definitions for the phase and group velocity, in multidimensional space for isotropic and lossless media is given in [56]. In [56] errors made in classical works on optics are pointed out regarding the group velocity in three dimensions. Therefore, we follow [56] for the definition of the phase and group velocity in multidimensional space.

From Eq. (3.1) it follows that in a homogeneous isotropic medium, each Cartesian component $V(r, t)$ of the field vectors $E$ and $H$ satisfies the homogeneous wave equation [16]

$$\nabla^2 V - \frac{1}{v^2} \frac{\partial^2 V}{\partial t^2} = 0, \quad (3.7)$$

where $r$ denotes the position vector of a point in space. We consider as a solution of Eq. (3.7) a time harmonic wave propagating in the direction of the wave vector $k = k\mathbf{u}$ ($\mathbf{u}$ is a unit vector)

$$E(r, t) = E_0(r)e^{-i(\omega t - k\cdot r + \Phi)} = E_0(r)e^{-i\Phi}e^{-i(\omega t - k\cdot r)}, \quad (3.8a)$$

$$H(r, t) = H_0(r)e^{-i(\omega t - k\cdot r + \Phi)} = H_0(r)e^{-i\Phi}e^{-i(\omega t - k\cdot r)}, \quad (3.8b)$$

where $\omega$ is called the angular frequency, $\Phi$ is a constant phase factor, and $E_0(r)$ and $H_0(r)$ are positive real scalar functions. Very often the amplitudes of the wave functions are considered to be complex, with their phase equal to the constant part $\Phi$ of the argument of the wave function. The waves have a frequency

$$f = \frac{\omega}{2\pi}, \quad (3.9)$$

and a wavelength

$$\lambda = \frac{v}{f} = v\frac{2\pi}{\omega}. \quad (3.10)$$
The length $k$ of the wave vector $\mathbf{k}$, which is by definition positive, is given by
\[
k = \frac{2\pi}{\lambda} = \frac{\omega}{c} = \frac{|n|\omega}{c} = \omega \sqrt{\varepsilon \mu}.
\] (3.11)

In optics $k$ is often called the wave number. The surfaces $\mathbf{k} \cdot \mathbf{r} = \text{const}$, that are surfaces of constant phase, are called wave fronts. In multidimensional space the phase velocity, that is the smallest speed at which the wave front propagates in the direction of the wave vector $\mathbf{k}$, is defined as \[56\]
\[v_p = \frac{\omega}{k} \mathbf{k}.
\] (3.12)
The magnitude of the phase velocity is
\[v_p = \frac{\omega}{k}.
\] (3.13)

Usually, a wave is a superposition of waves of slightly different frequencies and wave numbers. In such a case we call the wave a wave group or wave packet. To study the propagation of a wave packet we consider for the sake of simplicity and without loss of generality, two monochromatic plane waves of the same amplitude and slightly different frequencies and wave numbers
\[
E(r, t) = E_0 e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})} + E_0 e^{-i((\omega + \delta\omega) t - (\mathbf{k} + \delta\mathbf{k}) \cdot \mathbf{r})},
\] (3.14)

Eq. (3.14) can be rewritten as follows
\[
E(r, t) = 2E_0 \cos \left[ \frac{1}{2}(t\delta\omega - \mathbf{r} \cdot \delta\mathbf{k}) \right] e^{-i(\bar{\omega} t - \bar{\mathbf{k}} \cdot \mathbf{r})},
\] (3.15)

where $\bar{\omega} = \omega + \delta\omega/2$ and $\bar{\mathbf{k}} = \mathbf{k} + \delta\mathbf{k}/2$ are the mean frequency and mean wave vector, respectively.

The cosine term in Eq. (3.15) describes the variation with time and position of the amplitude of the wave packet. The surfaces $\delta\mathbf{k} \cdot \mathbf{r} - t\delta\omega = \text{const}$ are constant-amplitude surfaces or group fronts. The group-front velocity \[56\]
\[
v_{gf} = \frac{\delta\omega}{\delta k_x} \frac{\delta k_y}{\delta \omega} \frac{\delta k_z}{\delta \omega} = \frac{1}{2} \left[ \left( \frac{\delta k_x}{\delta \omega} \right)^2 + \left( \frac{\delta k_y}{\delta \omega} \right)^2 + \left( \frac{\delta k_z}{\delta \omega} \right)^2 \right]^{-1/2},
\] (3.16)
describes the propagation orthogonal to the group front and is the smallest speed at which the group front travels. The group-front velocity is generally not parallel to the phase velocity and has sometimes incorrectly been identified as the group velocity \[56\]. The definition of the group velocity is \[56\]
\[
v_g = \nabla k \omega.
\] (3.17)

In a normal dispersive, nondissipative and isotropic medium, the group velocity can be ex-
3.1. Conventional lossless dielectric materials

pressed as \[56\]

\[
v_g = \frac{\partial \omega}{\partial k} k.
\]  

(3.18)

The magnitude of the group velocity is

\[
v_g = \frac{\partial \omega}{\partial k}.
\]  

(3.19)

For linear wave propagation in a homogeneous, nondissipative media, it can be proven that the group velocity and energy velocity are equal (see for example [57, 58] and references therein). The group velocity thus identifies the direction and the speed of energy propagation. This is not true in general, since in regions of anomalous dispersion the magnitude of the group velocity may become greater than the speed of light or may become negative [59–63].

3.1.3 Phase and group refractive index

Sometimes the refractive index \(n\) is also called the phase refractive index \(n_p\), because it is related to the phase velocity \(v_p\). In terms of the frequency \(\omega\) of the wave and the wave vector \(k\) we have

\[
v_p = \frac{c}{|n_p|} = \frac{c}{|n|} = \frac{\omega}{k}.
\]  

(3.20)

The refractive index is thus always defined with respect to the phase velocity. In analogy to the phase refractive index also a group refractive index or group index \(n_g\) can be defined

\[
n_g = \frac{c}{v_g} = \frac{c}{\frac{\partial k}{\partial \omega}},
\]  

(3.21)

where use has been made of Eq. (3.19). If the medium is nondispersive, the phase and group velocity and hence the refractive and group index are the same. However, in general this is not the case. In a homogeneous isotropic dielectric medium the relation between the group index \(n_g\) and the refractive index \(n\) is given by

\[
n_g = c \frac{\partial k}{\partial \omega} = \frac{\partial}{\partial t} (\omega |n|) = |n| + \omega \frac{\partial |n|}{\partial \omega}.
\]  

(3.22)

3.1.4 Poynting vector

For a plane electromagnetic wave with wave vector \(k\) and angular frequency \(\omega\), the Maxwell’s and material equations reduce to

\[
k \times E = \omega \mu H,
\]  

(3.23a)

\[
k \times H = -\omega \varepsilon E.
\]  

(3.23b)
Projection on \( k \) gives

\[
\begin{align*}
    \mathbf{k} \cdot \mathbf{E} &= 0, \\
    \mathbf{k} \cdot \mathbf{H} &= 0.
\end{align*}
\]  

(3.24a) \hspace{1cm} (3.24b)

Hence the electric and magnetic field vectors lie in planes which are normal to the direction of propagation. Since for the materials discussed in this section \( \varepsilon \) and \( \mu \) are simultaneously positive, \( \mathbf{E}, \mathbf{H} \) and \( \mathbf{k} \) form a right-handed set of vectors. The energy flux associated with the electromagnetic wave is denoted by the Poynting vector

\[
\mathbf{S} = \mathbf{E} \times \mathbf{H}.
\]  

(3.25)

From Eq. (3.25) it follows that also \( \mathbf{S}, \mathbf{E} \) and \( \mathbf{H} \) form a right-handed set of vectors. Hence, \( \mathbf{S} \) and \( \mathbf{k} \) are parallel, that are positive multiples of the same unit vector \( \mathbf{u} \) and thus

\[
\mathbf{S} \cdot \mathbf{k} > 0.
\]  

(3.26)

As seen in Section 3.1.2, if the medium is not strongly dispersive the group velocity identifies the direction of energy propagation, and thus

\[
\mathbf{S} \cdot \mathbf{v}_g > 0.
\]  

(3.27)

From Eqs. (3.26) and (3.27) it follows that for homogeneous isotropic dielectric media with simultaneously positive \( \varepsilon \) and \( \mu \)

\[
\mathbf{v}_g \cdot \mathbf{k} > 0.
\]  

(3.28)

The group velocity is called positive, that is having the same sign as the wave vector.

If we now assume that the unit vector \( \mathbf{u} \) is defined through the Poynting vector \( \mathbf{S} \), we can write

\[
\mathbf{S} = \mathbf{S} \mathbf{u},
\]  

(3.29)

with \( S > 0 \) by definition. Since also \( \mathbf{k} \) is a positive multiple of \( \mathbf{u} \) we can write

\[
\mathbf{k} = \beta \mathbf{k} \mathbf{u} = \beta \frac{|n| \omega}{c} \mathbf{u},
\]  

(3.30)

with \( \beta = +1 \). Defining \( n = \beta |n| \) as the refractive index of the medium, it follows that homogeneous isotropic dielectric media with simultaneously positive permeability and permittivity have a positive refractive index. Rewriting the group velocity as

\[
\mathbf{v}_g = \beta \frac{\partial \omega}{\partial k} \mathbf{u},
\]  

(3.31)
3.1. Conventional lossless dielectric materials

and making use of Eq. (3.27) leads to the condition that

$$\beta \frac{\partial \omega}{\partial k} > 0.$$  \hfill (3.32)

Hence, for media that are not strongly dispersive, $\beta$ and $\frac{\partial \omega}{\partial k}$ always have the same sign. Rewriting the phase velocity as

$$v_p = \beta \frac{\omega}{k} u,$$ \hfill (3.33)

it can be concluded that

$$v_p \cdot k > 0.$$ \hfill (3.34)

Hence, in homogeneous isotropic dielectric media with simultaneously positive $\varepsilon$ and $\mu$ both the group velocity and the phase velocity are positive, that is having the same sign as the wave vector, or equivalently being parallel to the wave vector.

3.1.5 Reflection and refraction at an interface

When a plane wave falls on to an interface between two homogeneous isotropic media of different optical properties, it is split into two waves: a transmitted (refracted) wave proceeding into the second medium and a reflected wave propagating back into the first medium [16]. We assume that the reflected and refracted waves are also plane waves and derive expressions for their directions of propagation and their amplitudes.

We consider a plane wave with wave vector $k$ and frequency $\omega$ that is incident from a homogeneous isotropic medium with optical properties $\varepsilon$ and $\mu$. At the boundary with a second homogenous isotropic medium with optical properties $\hat{\varepsilon}$ and $\hat{\mu}$ the wave is split. The reflected

Figure 3.2: Incident plane wave with wave vector $k$ hits the plane interface $y = 0$ between two different media characterized by $\varepsilon$, $\mu$ and $\hat{\varepsilon}$, $\hat{\mu}$, respectively. $n$ denotes a unit normal vector.
and refracted plane waves have wave vectors and frequencies $\tilde{k}$, $\tilde{\omega}$ and $\hat{k}$, $\hat{\omega}$, respectively. We define $n$ as a unit normal directed from medium $\varepsilon$, $\mu$ into medium $\hat{\varepsilon}$, $\hat{\mu}$. At the boundary between the two media the time variation of all fields must be the same. Hence, at a point $r(x, y, z)$ on the boundary we have

$$\omega t - k \cdot r = \tilde{\omega} t - \tilde{k} \cdot r = \hat{\omega} t - \hat{k} \cdot r.$$  \hspace{1cm} (3.35)

If we take the boundary as the plane $y = 0$, Eq. (3.35) results in

$$\omega t - (k_x x + k_z z) = \tilde{\omega} t - (\tilde{k}_x x + \tilde{k}_z z) = \hat{\omega} t - (\hat{k}_x x + \hat{k}_z z).$$ \hspace{1cm} (3.36)

Since Eq. (3.36) must hold for all $t$ and all $x$ and $z$ on the boundary, we have

$$\omega = \tilde{\omega} = \hat{\omega}, \quad k_x = \tilde{k}_x = \hat{k}_x, \quad k_z = \tilde{k}_z = \hat{k}_z.$$ \hspace{1cm} (3.37)

Eq. (3.37) shows that both the reflected and refracted wave lie in the plane of incidence, that is the plane specified by the incident wave vector $k$ and the normal $n$. Taking the plane of incidence as the $xy$-plane gives $k_z = \tilde{k}_z = \hat{k}_z = 0$. A schematic picture is shown in Fig. 3.2. From Eq. (3.37) it follows that the tangential component of the incident wave vector is conserved upon reflection and refraction.

The energy flow associated with the incident electromagnetic wave is denoted by the Poynting vector

$$S = E \times H = \frac{1}{\omega \mu} (E \times (k \times E)) = \frac{E^2}{\omega \mu} k.$$ \hspace{1cm} (3.38)

From Eq. (3.38) it can be seen that for a medium with $\mu > 0$, $S \cdot k > 0$, a result already derived in Section 3.1.4 for materials with simultaneously positive $\varepsilon$ and $\mu$. Note that since

$$k_x^2 + k_y^2 = k_0^2 = \varepsilon \mu \omega^2,$$ \hspace{1cm} (3.39)

$\varepsilon$ and $\mu$ always have the same sign for homogeneous isotropic dielectric media. Also for the reflected wave $\tilde{S}$ and $\tilde{k}$ are parallel, that is $\tilde{S} \cdot \tilde{k} > 0$. If also the second medium has $\hat{\mu} > 0$, then $\hat{S} \cdot \hat{k} > 0$.

If the incident wave hits the boundary, the energy flux of the reflected and refracted wave is such that the energy flows away from the interface. The incident, reflected and refracted waves thus propagate as indicated in Fig. 3.3. If we define the angles $0 < \theta, \tilde{\theta}, \hat{\theta} \leq \pi/2$ as
Figure 3.3: Reflection and refraction of a plane wave at an interface between two homogeneous isotropic media of different optical properties, characterized by $\varepsilon, \mu > 0$ and $\hat{\varepsilon}, \hat{\mu} > 0$, respectively. $\mathbf{k}$ and $\mathbf{S}$ are the wave vector and Poynting vector of the incident wave, $\mathbf{\hat{k}}$ and $\mathbf{\hat{S}}$ are the wave vector and Poynting vector of the reflected wave and $\mathbf{\hat{\kappa}}$ and $\mathbf{\hat{\kappa}}$ are the wave vector and Poynting vector of the refracted wave. $\theta$, $\tilde{\theta}$ and $\hat{\theta}$ correspond to the angle of incidence, the angle of reflection and the angle of refraction, respectively. The angles are measured in a counterclockwise or positive direction.

From Eqs. (3.37) and (3.40) it follows that
\[
\theta = \tilde{\theta},
\]  
(3.41)

and
\[
\frac{\sin \theta}{\sin \tilde{\theta}} = \frac{\hat{k}}{k} = \frac{|\hat{n}|}{|n|},
\]  
(3.42)

where use has been made of $\hat{k} = k = |n|\omega/c$. Relation (3.41), together with the statement that the reflected wave vector is in the plane of incidence, constitute the law of reflection [16].
3. Light propagation in dielectric materials

Relation (3.42), together with the statement that the refracted wave vector is in the plane of incidence, constitute the law of refraction or Snell’s law \[16\].

We now consider the amplitudes of the reflected and refracted waves. The electric and magnetic field vectors obey the Maxwell equations and material equations. Across the boundary of the two homogeneous isotropic dielectric media the tangential component of $E$ and $H$ should be continuous \[16\]. Hence we must have

\[
\mathbf{n} \times (\mathbf{E} + \tilde{\mathbf{E}}) = \mathbf{n} \times \tilde{\mathbf{E}},
\]
(3.43a)

\[
\mathbf{n} \times (\mathbf{H} + \tilde{\mathbf{H}}) = \mathbf{n} \times \tilde{\mathbf{H}},
\]
(3.43b)

and thus

\[
E_x + \tilde{E}_x = \tilde{E}_x,
\]
(3.44a)

\[
E_z + \tilde{E}_z = \tilde{E}_z,
\]
(3.44b)

\[
H_x + \tilde{H}_x = \tilde{H}_x,
\]
(3.44c)

\[
H_z + \tilde{H}_z = \tilde{H}_z.
\]
(3.44d)

Also the normal components of $D$ and $B$ should be continuous across the boundary \[16\]

\[
(\mathbf{D} + \tilde{\mathbf{D}}) \cdot \mathbf{n} = \tilde{\mathbf{D}} \cdot \mathbf{n},
\]
(3.45a)

\[
(\mathbf{B} + \tilde{\mathbf{B}}) \cdot \mathbf{n} = \tilde{\mathbf{B}} \cdot \mathbf{n},
\]
(3.45b)

and by making use of Eq. (2.3)

\[
\varepsilon (E_y + \tilde{E}_y) = \tilde{\varepsilon} \tilde{E}_y,
\]
(3.46a)

\[
\mu (H_y + \tilde{H}_y) = \tilde{\mu} \tilde{H}_y.
\]
(3.46b)

From Eqs. (3.23b), (3.44a), (3.44d) and the fact that $k_z = \tilde{k}_z = \hat{k}_z = 0$ it follows that

\[
\frac{\tilde{H}_z}{\tilde{H}_z} = \frac{\varepsilon (k_y - \tilde{k}_y)}{\varepsilon k_y - \tilde{\varepsilon} k_y}.
\]
(3.47)

For the case $\varepsilon, \mu > 0$ and $\varepsilon, \tilde{\mu} > 0$, $\tilde{k}_y = -k_y = -|n|\omega/c \cos \theta$ and $\tilde{\varepsilon} k_y = |n|\omega/c \cos \tilde{\theta}$ (see Eq. (3.40)). Hence, for the special case of a conventional homogeneous dielectric medium with $\mu = \tilde{\mu} = 1$, $n = \sqrt{\varepsilon}$ and $\tilde{n} = \sqrt{\varepsilon}$, we have \[16\]

\[
\frac{\tilde{H}_z}{\tilde{H}_z} = \frac{2|\tilde{n}| \cos \theta}{|n| \cos \theta + |\tilde{n}| \cos \tilde{\theta}}.
\]
(3.48)

Using Eqs. (3.37), (3.23b), (3.24b), (3.44b), (3.44c) and the fact that $k_z = \tilde{k}_z = \hat{k}_z = 0$ we
obtain

\[
\frac{\hat{H}_x}{H_x} = \frac{\hat{\varepsilon}k_y (k_x^2 - k_y \tilde{k}_y)(k_y - \tilde{k}_y)}{k_y \hat{\varepsilon}k_y (k_y^2 + k_x^2) - \varepsilon \tilde{k}_y^2 k_y},
\]  

(3.49)

where \( \tilde{k}^2 = \hat{k}_x^2 + \hat{k}_y^2 = \omega^2 \hat{\varepsilon} \hat{\mu} \). Using the relations in Eq. (3.40) for materials with \( \mu = \hat{\mu} = 1 \), \( n = \sqrt{\hat{\varepsilon}} \) and \( \hat{n} = \sqrt{\hat{\varepsilon}} \), we find [16]

\[
\frac{\hat{H}_x}{H_x} = \frac{2|\hat{n}| \cos \hat{\theta}}{|n| \cos \theta + |\hat{n}| \cos \hat{\theta}}.
\]  

(3.50)

The expression for \( \frac{\hat{H}_y}{H_y} \) follows from Eq. (3.24b),

\[
\frac{\hat{H}_y}{H_y} = \frac{\hat{k}_x k_y \hat{H}_x}{k_y \hat{k}_x H_x}.
\]  

(3.51)

Using the relations in Eq. (3.40) for the case \( \varepsilon, \mu > 0 \) and \( \hat{\varepsilon}, \hat{\mu} > 0 \), Eq. (3.51) can be rewritten as

\[
\frac{\hat{H}_y}{H_y} = \frac{\sin \hat{\theta} \cos \theta \hat{H}_x}{\sin \theta \cos \hat{\theta} H_x}.
\]  

(3.52)

The relative amplitudes for the reflected waves can be found by making use of Eqs. (3.44c), (3.44d) and (3.46b),

\[
\frac{\hat{H}_z}{H_z} = \hat{H}_z - 1,
\]  

(3.53a)

\[
\frac{\hat{H}_x}{H_x} = \hat{H}_x - 1,
\]  

(3.53b)

\[
\frac{\hat{H}_y}{H_y} = \hat{\mu} \frac{\hat{H}_y}{\mu H_y} - 1.
\]  

(3.53c)

The relative amplitudes for the \( E \) fields can be found from the ones of the \( H \) fields by interchanging the role of \( \varepsilon \) and \( \mu \) and \( \hat{\varepsilon} \) and \( \hat{\mu} \).

### 3.1.6 Total internal reflection

In the optical frequency regime, the range of refractive indices of materials is limited typically between 1 and 4. From Snell’s law it can be seen that if light crosses an interface into a medium with a higher index of refraction, the light bends towards the normal, as illustrated in Fig. 3.4a. If light travels across an interface from a material with higher refractive index to a material with lower refractive index, then it will bend away from the normal, as can be seen from Fig. 3.4b. For both cases \( n < \hat{n} \) and \( n > \hat{n} \), the refracted beam and the incident beam are positioned at opposite sides of the normal. The case \( n > \hat{n} \) is somewhat special.
Figure 3.4: Illustration of the refraction of light at the interface between two homogeneous isotropic media with refractive indices \( n > 0 \) and \( \hat{n} > 0 \). \( k \) is the incident wave vector and \( \hat{k} \) is the refracted wave vector. \( \theta \) corresponds to the angle of incidence and \( \hat{\theta} \) to the refracted angle. The angles are measured in a counterclockwise or positive direction.

At some angle, known as the critical angle \( \theta_c \), light traveling from medium 1 with refractive index \( n \) to medium 2 with refractive index \( \hat{n} \) will be refracted at \( 90^\circ \), that is refraction along the interface. This can be seen as follows. From the relations

\[
\hat{k}_y^2 = \left( \frac{\hat{\varepsilon} \hat{\mu}}{\varepsilon \mu} - 1 \right) k_x^2 + \frac{\hat{\varepsilon} \hat{\mu}}{\varepsilon \mu} k_y^2,
\]

where use has been made of the fact that the tangential component of the incident wave vector is conserved upon refraction, that is \( \hat{k}_x = k_x \). If a wave should propagate in medium 2, then \( \hat{k}_y \) should be real and thus

\[
\left( \frac{\hat{\varepsilon} \hat{\mu}}{\varepsilon \mu} - 1 \right) k_x^2 + \frac{\hat{\varepsilon} \hat{\mu}}{\varepsilon \mu} k_y^2 > 0.
\]

Note that if \( \hat{\varepsilon} \hat{\mu} > \varepsilon \mu \) (or \( \hat{n} > n \)), then condition (3.57) is always fulfilled. Substituting the expressions for \( k_x \) and \( k_y \) from Eq. (3.40) into Eq. (3.57) gives

\[
\sin^2 \theta < \frac{\hat{\varepsilon} \hat{\mu}}{\varepsilon \mu}.
\]

Thus, if the angle of incidence is larger than \( \theta_c = \arcsin(\hat{n}/n) \), the incident light beam will not pass through the second medium at all. All the light is totally reflected off the interface.
3.1. Conventional lossless dielectric materials

3.1.7 Propagation through a slab

Experimentally, the refractive index of a material can be determined from the apparent displacement $L$ of an electromagnetic wave when it travels through a slab of thickness $D$ of this material

$$\hat{n} = \frac{n \sin \theta}{\sin(\arctan(L/D))}, \quad (3.59)$$

as illustrated in Fig. 3.5ab for the cases $n < \hat{n}$ and $n > \hat{n}$, respectively. As can be seen from Fig. 3.5, the shift $L$ is always much larger for the case $n > \hat{n}$ than for the case $n < \hat{n}$.

3.1.8 FDTD simulation of refraction in a homogeneous isotropic slab

Using our finite-difference time domain (FDTD) simulation code described in Chapter 2 we simulate the refraction of a light beam in a slab of a homogeneous, isotropic dielectric material with refractive index $\hat{n}$. We assume that the surrounding medium is vacuum ($n = 1$). We simulate two illustrative cases, one for $\hat{n} = 2$ and one for $\hat{n} = 0.8$. We consider a slab of dimension $12\lambda \times 40\lambda$ and optical parameters $\hat{\varepsilon} = 4, \hat{\mu} = 1$ ($\hat{n} = 2$) and $\hat{\varepsilon} = 0.64, \hat{\mu} = 1$ ($\hat{n} = 0.8$), respectively. The total simulation area has dimensions $L_x = 44\lambda$ and $L_y = 40\lambda$. The boundaries of the box are absorbing. We discretize the space in a square grid with lattice spacing $\delta = 0.02\lambda$. This results in a total number of 440000 lattice points. We use a time step $\delta t = 0.002\lambda/c$. For these values of the parameters $\delta$ and $\delta t$ the simulation results are very accurate.
Figure 3.6: FDTD simulation results for the propagation of an electromagnetic wave (TM mode) through a slab. The snapshots are taken at $t = 50\lambda/c$. The arrows indicate the direction of propagation according to Snell’s law and the law of reflection. (a): $\hat{n} = 2, \theta = 26.57^\circ$; (b): $\hat{n} = 2, \theta = 45^\circ$; (c): $\hat{n} = 0.8, \theta = 26.57^\circ$; (d): $\hat{n} = 0.8, \theta = 63.43^\circ$. For the other simulation parameters we refer to the text.

In front of the slab, we put a line source, modeled by

$$J(r, t) = \mathbf{O} J(r) e^{-C_0 |r-r_0|^2/W^2} \sin(\Omega t),$$

(3.60)

where $\mathbf{O}$ defines the direction of the electric (TM mode) or magnetic (TE mode) current and $\Omega$ the angular frequency of the line source, $J(r)$ defines the spatial distribution of the intensity and angle of incidence $\theta$, $C_0$ is a constant, $r_0$ is the center of the line source and $W$ is the half length of the line source. At $t = 0$, the source starts gradually emitting a TM wave or a TE wave.
3.1. Conventional lossless dielectric materials

Fig. 3.7: Same as Fig. 3.6 but for a TE wave.

Fig. 3.6 shows the simulation results for a TM wave. The parameters for the line source are $C_0 = 5, W = 8\lambda, r_0 = (10\lambda, 10\lambda), \Omega = 2\pi c/\lambda$. The snapshots show $E_z^2$ and are taken at $t = 50\lambda/c$. Figs. 3.6a,b depict the results for $n = 2, \theta = 26.57^\circ$ and $\hat{n} = 2, \theta = 45^\circ$, respectively. For both examples the propagation of the refracted and reflected wave exactly follows Snell’s law and the law of reflection, as indicated by the arrows. Figs. 3.6c,d show simulation results for $\hat{n} = 0.8$. In this case, the incident light will be totally reflected off the interface if the angle of incidence is larger than $\theta_c = 53.13^\circ$. This effect is illustrated in Fig. 3.6d, where $\theta = 63.43^\circ$. If $\theta < \theta_c$, a reflected and a refracted beam exist, just as in the case $n < \hat{n}$. An example is shown in Fig. 3.6c, where $\theta = 26.57^\circ$. From Fig. 3.6c,d it can be concluded that also for the case $\hat{n} < n$, the simulated light propagation exactly follows Snell’s law and the law of reflection.
In Fig. 3.7 we show simulation results for a line source emitting a TE wave. The simulation parameters are taken to be exactly the same as the ones used in the simulations to produce the results depicted in Fig. 3.6. As seen from Fig. 3.7 also the propagation of the TE wave exactly follows Snell’s law and the law of reflection.

In summary, the simulation results presented in Fig. 3.6 and Fig. 3.7 demonstrate that our FDTD simulation code correctly simulates the propagation of light, generated by a line source, through a homogeneous isotropic slab of material with $\hat{\varepsilon}, \hat{\mu} > 0$.

3.2 Dielectrics with negative permeability and permittivity

3.2.1 Refractive index, phase and group velocity

If $\varepsilon < 0$ and $\mu < 0$, then it follows from Eq. (3.23) that $E$, $H$ and $k$ form a left-handed set of vectors. According to Eq. (3.25), the Poynting vector $S$ always forms a right-handed set with the vectors $E$ and $H$. Accordingly, $S$ and $k$ are antiparallel, that is $S$ and $k$ can be written as $S = S\hat{u}$ and $k = \beta k\hat{u}$ with $\beta = -1$, respectively. Hence, $S \cdot k < 0$. Since in weakly dispersive media $S \cdot v_g > 0$, the sign of $v_g \cdot k$ is equivalent to the sign of $S \cdot k$, which in this case is negative. The group velocity is called negative, that is having the opposite sign as the wave vector. From Eq. (3.32) it follows that $\partial\omega/\partial k < 0$ and hence $n_g < 0$. Using Eqs. (3.29) and (3.30) with $\beta = -1$ it can be seen that the sign of the refractive index $n$ is the sign of $S \cdot k$, and thus also of $v_g \cdot k$. Thus, homogeneous isotropic dielectric media with simultaneously negative permeability and permittivity have a negative refractive index. Note that independent of the sign of $\beta$, or equivalently independent of the sign of $n$, $v_p \cdot k > 0$, as can be seen from Eqs. (3.30) and (3.34). Therefore, in homogeneous isotropic dielectric media with a negative refractive index, the group velocity is negative (that is having the opposite sign as the wave vector) while the phase velocity is positive (that is having the same sign as the wave vector).

A summary of the above findings and a comparison to the ones for the case $\varepsilon > 0, \mu > 0$ is given in Table 3.1.

The consequences of the fact that for media with $\varepsilon < 0$ and $\mu < 0$, the wave vector and the Poynting vector are antiparallel are a reversed Doppler effect [64], a reversed Vavilov-Cerenkov effect [64], negative refraction [64], imaging by a flat lens, the replacement of the radiation pressure characteristic of ordinary substances by a radiation tension or attraction [64], and open cavity formation [3, 17].

In the literature on materials that show negative refraction, there sometimes is confusion about the definition of the refractive index related to the observed negative refraction. Therefore we briefly explain the relation of the phase and group refractive indices $n_p$ and $n_g$ to negative refraction.
3.2. Dielectrics with negative permeability and permittivity

Table 3.1: Phase and group velocities and their associated phase and group refractive indices for homogeneous isotropic dielectric materials.

<table>
<thead>
<tr>
<th>$\varepsilon &gt; 0, \mu &gt; 0$</th>
<th>$\varepsilon &lt; 0, \mu &lt; 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbf{S} \cdot \mathbf{k} &gt; 0$</td>
<td>$\mathbf{S} \cdot \mathbf{k} &lt; 0$</td>
</tr>
<tr>
<td>$\mathbf{S} \cdot \mathbf{v}_g &gt; 0$</td>
<td>$\mathbf{S} \cdot \mathbf{v}_g &gt; 0$</td>
</tr>
<tr>
<td>$\mathbf{v}_g \cdot \mathbf{k} &gt; 0$</td>
<td>$\mathbf{v}_g \cdot \mathbf{k} &lt; 0$</td>
</tr>
<tr>
<td>$n_p = n &gt; 0$</td>
<td>$n_p = n &lt; 0$</td>
</tr>
<tr>
<td>$n_g &gt; 0$</td>
<td>$n_g &lt; 0$</td>
</tr>
<tr>
<td>$\mathbf{v}_p \cdot \mathbf{k} &gt; 0$</td>
<td>$\mathbf{v}_p \cdot \mathbf{k} &gt; 0$</td>
</tr>
</tbody>
</table>

Negative refraction of a wave propagating from one medium to another is said to be observed when the wave in the second medium appears at the same side of the normal to the interface as in the first medium. As described above, in a homogeneous isotropic dielectric medium with normal dispersion, negative refraction occurs when the (phase) refractive index is negative. It was also shown that $n_g < 0$ when $n_p < 0$. However, note that because in this case the group velocity corresponds to the energy velocity, which is less than $c$, $|n_g|$ has to be larger than one.

Negative refraction can for example also be observed in anisotropic dispersive media. For anisotropic dispersion cases, $\mathbf{v}_g$ and $\mathbf{k}$ are not along the same direction. In that case the sign of $n_g$ is chosen to manifest the sign of refraction at the interface and therefore $n_g$ has the sign of $(\mathbf{v}_g \cdot \mathbf{k})_x$, where $x$ denotes the direction along the interface and $\mathbf{k}$ the incident wave vector \[65]\). It can be seen that $(\mathbf{v}_g \cdot \mathbf{k})_x < 0$, while $(\mathbf{v}_g \cdot \mathbf{k}) > 0$ and thus $n_p > 0$. All possible combinations of signs for the phase and group refractive indices are possible \[65]\.

In the case of normal dispersion $n_p = n$ can be used in Snell’s law to determine the propagation angle of the wave \[65]\, also if $n < 0$ (see Section 3.2.3). However, $n_g$ cannot be used in Snell’s formula to obtain the propagation direction of the wave \[65]\). If negatively appearing refraction is observed, it should be carefully checked whether it is caused by a negative refractive index of an isotropic dielectric medium or that it is due to anisotropy of the medium (see for example \[66]\).

3.2.2 History and terminology

The first theoretical study of wave propagation in materials for which $\varepsilon$ and $\mu$ are simultaneously negative has often been attributed to Veselago, who published his work in 1967 \[64]\ (Translation from the original Russian version in Usp. Fiz. Nauk. 92, 517 (1967). This year was mislabeled in the translation as 1964). Because for media with $\varepsilon < 0$ and $\mu < 0$ the vectors $\mathbf{E}$, $\mathbf{H}$ and $\mathbf{k}$ form a left-handed set of vectors, Veselago referred to these materials
as left-handed materials. The conventional lossless dielectric media with \( \varepsilon > 0, \mu > 0 \), he named right-handed materials. Unfortunately, these names are not well-chosen. The left or right handedness also refers to the molecular structure of chiral materials that are often studied in electromagnetics research \[67\]. Therefore several other names are used in the literature. We only mention the most common ones.

Since for a plane wave in a homogeneous isotropic medium with \( \varepsilon < 0 \) and \( \mu < 0 \), the Poynting vector and wave vector are antiparallel (see Section 3.2.1). Lindell et al. \[68, 69\] suggested the name backward-wave media. They were however not the first to use this name. Already at the end of the fifties and the beginning of the sixties backward waves were known to exist in some periodic structures with applications to microwave amplifiers, oscillators and antennas \[70–73\]. Backward-waves have also been generated in continuous structures like a sheet of plasma \[74\]. However, as mentioned on the website of Moroz \[61\], Lamb and Schuster in 1904 may even have been the first to study the possibility of a negative group velocity, that is having the opposite sign to the wave vector, and thus to study the existence of backward-waves. Lamb studied mechanical systems, free from dissipation, in which the group velocity can become negative \[62\]. In his paper, Lamb mentioned that Schuster proposed to him the possibility of a negative group velocity and that Schuster pointed out that the optical formulae relating to anomalous dispersion indicate a negative group velocity for certain portions of the spectrum lying within the regions of special absorption. Also Pocklington mentioned in 1905 waves propagating toward the source of disturbance in a mechanical system \[75\]. Another name to media with \( \varepsilon < 0 \) and \( \mu < 0 \) was given by Ziolkowski et al. \[76, 77\], who denoted these media as double negative materials. On the other hand, media with both positive permittivity and permeability they denoted as double positive media. Since homogeneous isotropic dielectric media with \( \varepsilon < 0 \) and \( \mu < 0 \) have a negative refractive index (see Section 3.2.1), these materials are also often called negative index materials (see for example \[78–80\]). Materials with a positive refractive index are then called positive index materials.

Renewed interest to the negative index materials after Veselago’s proposal in 1967 is usually attributed to Pendry who in 2000 pointed out that negative refraction makes a perfect lens \[81\]. Recently, a lot of experimental efforts are put in finding materials that have a negative refractive index. In this respect it is also worthwhile to mention the work by Silin on the possibility of creating plane-parallel lenses, which appeared in 1978 \[82\]. With his paper, Silin wanted to draw attention to the possibility of creating new type of optical elements using media with unusual dispersion laws and to stimulate the search for media with unusual dispersion laws. Silin also refers to the theoretical and experimental investigation of the law of refraction for media with negative dispersion by Mandelshtam in the late forties \[83, 84\]. In 1972, Silin also published an article on artificial dielectrics \[85\]. Artificial dielectrics have complicated dispersion characteristics. They are encountered in media in the form of periodic structures of metal or dielectric bundles and they were widely used in superhigh-frequency
3.2. Dielectrics with negative permeability and permittivity

3.2.3 Reflection and refraction at an interface between a positive and a negative index material

We follow the same procedure as described in Section 3.1.5 to study the propagation of a plane wave with wave vector \( \mathbf{k} \) and frequency \( \omega \) falling on to an interface between a homogeneous isotropic medium with optical properties \( \varepsilon > 0, \mu > 0 \) and a homogeneous isotropic medium with optical properties \( \varepsilon < 0, \mu < 0 \). At the boundary the wave is split. The reflected and refracted plane waves have wave vectors and frequencies \( \tilde{\mathbf{k}}, \tilde{\omega} \) and \( \hat{\mathbf{k}}, \hat{\omega} \), respectively. As discussed in Section 3.1.5 the tangential component of the incident wave vector is conserved upon reflection and refraction. This is independent from the sign of \( \varepsilon \) and \( \mu \), whether they are both positive or negative. From Eq. (3.38) it follows that if \( \varepsilon > 0, \mu > 0 \) and \( \varepsilon < 0, \mu < 0 \), then \( \mathbf{S} \cdot \mathbf{k} > 0, \tilde{\mathbf{S}} \cdot \tilde{\mathbf{k}} > 0 \) and \( \hat{\mathbf{S}} \cdot \hat{\mathbf{k}} < 0 \). Note that because \( \tilde{\mathbf{S}} \cdot \tilde{\mathbf{k}} < 0 \) also \( \hat{n} < 0 \) (see Table 3.1). Since, if the incident wave hits the boundary, the energy flux of the reflected and refracted wave is such that the energy flows away from the interface, the incident, reflected and refracted waves propagate as indicated in Fig. 3.8. As can be seen from Fig. 3.8 the refracted and the incident beam are positioned at the same side of the normal to the interface.
If we define the angles $0 \leq \theta, \tilde{\theta}, \hat{\theta} \leq \pi/2$ as indicated in Fig. 3.8, we have

$$
k_x = k \cos(\frac{\pi}{2} - \theta) = k \sin \theta, \quad (3.61a)
$$

$$
k_y = k \sin(\frac{\pi}{2} - \theta) = k \cos \theta, \quad (3.61b)
$$

$$
\tilde{k}_x = \tilde{k} \cos(\frac{3\pi}{2} + \tilde{\theta}) = \tilde{k} \sin \tilde{\theta}, \quad (3.61c)
$$

$$
\tilde{k}_y = \tilde{k} \sin(\frac{3\pi}{2} + \tilde{\theta}) = -\tilde{k} \cos \tilde{\theta}, \quad (3.61d)
$$

$$
\hat{k}_x = \hat{k} \cos(\frac{3\pi}{2} + \hat{\theta}) = \hat{k} \sin \hat{\theta}, \quad (3.61e)
$$

$$
\hat{k}_y = \hat{k} \sin(\frac{3\pi}{2} + \hat{\theta}) = -\hat{k} \cos \hat{\theta}. \quad (3.61f)
$$

From Eqs. (3.37) and (3.61) it follows that

$$
\tilde{\theta} = \theta \quad (3.62)
$$

and

$$
\frac{\sin \theta}{\sin \tilde{\theta}} = \frac{\hat{k}}{\tilde{k}} = \frac{|\hat{n}|}{|\tilde{n}|} = \frac{\hat{n} \beta}{\tilde{n} \beta} \quad (3.63)
$$

where use have been made of

$$
\tilde{k} = k = \frac{|\tilde{n}| \omega}{c}, \quad \text{and} \quad \hat{k} = \frac{|\hat{n}| \omega}{c}. \quad (3.64)
$$
3.2. Dielectrics with negative permeability and permittivity

Note that in Eq. (3.63) \( n > 0, \beta = +1 \) and \( \hat{n} < 0, \beta = -1 \). The ratios in Eq. (3.63) should be positive, since a ratio of two vector lengths is involved and vector lengths are by definition positive. However, in the literature it is often mentioned that Snell’s law

\[
\frac{\sin \theta}{\sin \hat{\theta}} = \frac{\hat{n}}{n},
\]

(3.65)

can still be used if the observed refracted beam lies on the same side of the normal to the interface as the incident beam does and that in that case a negative refractive index is found for the medium \( \hat{n} < 0 \) while \( n > 0 \). In that case, however it is assumed that the angle of refraction is equal to minus the refraction angle for the case of normal refraction, as indicated in Fig. 3.9 (see also [64]). As a result \( \hat{\theta} < 0, 0 < |\hat{\theta}| \leq \pi/2 \) and Eq. (3.63) can be rewritten as

\[
\frac{\sin \theta}{\sin \hat{\theta}} = \frac{-\hat{k}}{k} = -\frac{|\hat{n}|}{|n|} = -\frac{\hat{n} \beta}{\beta n} = \frac{\hat{n}}{n},
\]

(3.66)

with \( \hat{n} < 0 \) and \( n > 0 \).

The amplitudes of the reflected and refracted waves can be found using the expressions (3.50), (3.52), (3.48) and (3.53) derived in Section 3.1.5. For the case that \( \hat{\varepsilon} = -\varepsilon \) and \( \hat{\mu} = -\mu \), there is no reflection at the interface. The angle of refraction is equal to the angle of incidence and the refracted beam is positioned at the same side of the normal to the interface as the incident beam is. Note that if \( |\hat{n}| < |n| \), the phenomenon of total internal reflection (see Section 3.1.6) can still be observed. This phenomenon occurs independent of the sign of \( \hat{n} \).

3.2.4 Subwavelength imaging

One of the interesting properties of negative index materials is their ability to focus light. Conventional lenses are convex. They have a converging effect on light rays. The resolution of a conventional (convex) lens is always limited by the wavelength of the light. A light beam cannot be focused to a spot with a diameter smaller than half of the wavelength of the light. In 1967, Veselago has shown theoretically that a convex lens made of a negative index material would be diverging light and that a concave lens made of negative index material would be converging light [64]. This behavior is thus opposite to the behavior observed for convex and concave lenses made of positive index materials. Veselago also noted that a flat plate of thickness \( D \) made of negative index material with \( \hat{n} = -1 \) and situated in vacuum can focus radiation from a point source \( P \) positioned at a distance \( L < D \) from one side of the plate to a point \( P' \) located at a distance \( D - L \) from the other side of the plate (see Fig. 3.10) [64]. As can be seen from Fig. 3.10, also an image inside the slab is formed. However, as Veselago has remarked, the flat plate, unlike a conventional lens, will not focus at a point a beam of rays coming from infinity [64].
3. Light propagation in dielectric materials

![Diagram of imaging by a flat slab of thickness $D$ of negative index material with $\hat{n} = -1$ and surrounded by vacuum. A point source $P$ is positioned at a distance $L$ from the left surface of the slab. A “perfect” image of the source can be observed in the point $P'$, located at a distance $D - L$ from the right surface of the slab.](image)

**Figure 3.10:** Imaging by a flat slab of thickness $D$ of negative index material with $\hat{n} = -1$ and surrounded by vacuum. A point source $P$ is positioned at a distance $L$ from the left surface of the slab. A “perfect” image of the source can be observed in the point $P'$, located at a distance $D - L$ from the right surface of the slab.

In 1978, Silin showed that plane-parallel lenses can be constructed on the basis of media with negative dispersion [82]. He demonstrated that it is possible to choose an isotropic medium such that monochromatic aberrations can be eliminated for such lenses [82]. In 2000, Pendry further pointed out that flat slabs of negative index material with $\hat{n} = -1$ and surrounded by vacuum make perfect lenses or superlenses, since both propagating and evanescent waves contribute to the resolution of the image [81]. These lenses are thus predicted to have sub-wavelength resolution. Because Pendry also demonstrated by means of simulations that such a lens operating at the frequency of visible light can be physically realized in the form of a thin slab of silver, a lot of research has been performed on negative index materials and superlenses since 2000. However, limitations of the superlensing effect have also been subject of debate [86–92]. In 2001, Ziolkowski *et al.* have shown analytically that the perfect lens effect exists only for a negative index material with $\varepsilon = \mu = -1$ that is both lossless and nondispersive [76]. The perfect lens effect was shown not to exist for any realistic dispersive, lossy negative index material. The simulation results of Loschialpo *et al.* [93, 94] do not support a perfect lens, as postulated by Pendry [81], either.

### 3.2.5 Physical realization of negative index materials

The search for media with a negative refractive index has led to the fabrication of the so-called metamaterials [78, 95, 96]. Metamaterials are artificial materials that consist of a collection of repeated objects whose size and spacing are much smaller than the electromagnetic wavelength of interest. As such the inhomogeneous composite can be described by a homogeneous material with effective material properties $\varepsilon_{\text{eff}}$ and $\mu_{\text{eff}}$ [78, 95, 96]. The
properties of the complex material can thus be summarized by an effective permittivity and permeability, which is a great simplification.

Negative permittivities can be obtained in cut-wire media \[97, 98\]. In 1999, a variety of structures was proposed that could form magnetic metamaterials \[99\]. Those structures, splitting resonators, consisting of loops or tubes of conductor with a gap inserted, can lead to a negative permeability. Soon after the introduction of the split-ring resonator media by Pendry in 1999 \[99\], composite wire and split ring resonator structures were fabricated for which a negative \(\varepsilon_{\text{eff}}\) and \(\mu_{\text{eff}}\) was predicted for a frequency region in the microwave regime \[100, 101\]. The first experiment, showing negative refraction in a prism of metamaterial designed to have a negative effective refractive index \(n_{\text{eff}}\) in the microwave frequency regime, was performed in 2001 by Shelby et al. \[102\].

Because the physical realization of materials with a negative refractive index remained questioned \[53, 103\], in 2003 Houck et al. produced new experimental evidence showing that transmission through a metamaterial wedge sample, similar to the one in the first demonstration, is in accordance to Snell’s law with a negative refractive index \[104\]. In addition, the experiment gave preliminary evidence for the focusing properties of a flat slab of negative index material. In the same year, results of Snell’s law experiment on a negative index metamaterial wedge were reported \[105\]. In contrast to the two previous experiments, in which two-dimensional composite wire and split ring resonator structures were used, in this experiment a one-dimensional negative index material structure was used. Also this experiment supported the observation reported by Shelby et al. \[102\]. Recently, measurements on flat slabs of composite wire and split ring resonator negative index materials have been presented that show focusing inside and outside the metamaterial \[80\]. Additionally, a linear dependence of the focal length on the frequency was demonstrated \[80\]. However, focusing with subwavelength resolution using such a composite wire split ring resonator lens remained experimentally elusive \[80\]. Although, results have been reported that a planar negative index transmission-line-lens can form images that overcome the diffraction limit \[106\]. Recently, Pendry proposed chiral materials as an alternative to produce negative index materials \[107\].

A second approach to construct negative index metamaterials is based on the concept of transmission line structures, which are common in electrical engineering applications. This approach has been described by Eleftheriades et al. in 2002 \[108\]. The transmission-line structures consist of two-dimensional transmission-line (TL) grids loaded with series capacitors (C) and shunt inductors (L) \[108\]. Using this L-C loaded TL approach, negative refraction \[108\] and focusing was demonstrated at microwave frequencies \[108, 109\]. Radiating versions of these media have been used to experimentally demonstrate backward-wave radiation in free space, a characteristic analogue to reversed Cherenkov radiation \[110\]. The focusing reported in \[108, 109\] was obtained by lenses utilizing a single interface between a left-handed medium and a homogeneous dielectric. Imaging beyond the diffraction limit
could not clearly be observed with these lenses. Subsequently, planar slabs (having two interfaces) of L-C loaded TL left-handed media were shown theoretically to enhance the amplitudes of evanescent waves [111, 112] and to focus propagation waves with subwavelength resolution [112]. In a later study, these theoretical findings were confirmed experimentally [106].

A third approach to obtain the phenomena of negative refraction and imaging by a planar surface is to use photonic crystals. In contrast to the metamaterials described above, photonic crystals are periodic structures typically composed of insulators. Therefore they can exhibit low losses, even at the higher (optical) frequencies, a property that can be important in applications. In photonic crystals, the size and spacing of the scattering elements are on the order of the electromagnetic wavelength of interest. Therefore a photonic crystal cannot be regarded as a homogeneous medium and its properties cannot be described by an effective permittivity and permeability. Nevertheless, in 2000 Notomi has shown theoretically that photonic crystals near the band gap frequency behave as if they have an effective refractive index [3]. For some frequency regions this effective refractive index can be negative [3]. As a result in these frequency regions, photonic crystals can exhibit the same phenomena as observed in negative index materials, including negative refraction and imaging by a planar surface [3, 17]. In 2003, negative refraction was experimentally observed in a two-dimensional photonic crystal operating in the microwave regime [113–115]. Also subwavelength imaging has been demonstrated in 2003 [114, 115]. More experimental evidence of negative refraction [116–118] and subwavelength imaging [118–124] in photonic crystals followed rapidly. Note that the experimentally observed negative refraction and subwavelength imaging is not always due to a negative effective refractive index, but due to anisotropy. This is the case for the negative refraction observed in [113–115, 123]. Moreover, all this theoretical and experimental evidence for negative refraction and subwavelength imaging is for two-dimensional photonic crystals. Although these two-dimensional crystals are very important for the investigation of negative refraction and flat lenses with subwavelength resolution, the realization of such lenses in three dimensions is of significant importance for many applications. Luo et al. [125] and Ao et al. [126] proposed and theoretically investigated such lenses, made of three-dimensional photonic crystals with BCC lattice symmetry. In 2005, Lu et al. [127] have experimentally demonstrated for the first time subwavelength resolution imaging at microwave frequencies by a three-dimensional photonic crystal flat lens. The photonic crystal is a BCC structure similar to the one proposed by Luo et al. [125].

In [66], Ye questions whether the current evidence for negative index materials and the related negative refraction is sufficient or conclusive, without criticizing the experimental evidence and theoretical analysis. Ye’s conclusion is that the current experimental evidence is not sufficient to conclude that negative index materials have been fabricated and that a detailed exploration has to be carried out with regard to all aspects of negative refraction [66].
3.3 Photonic crystals

As discussed above, metamaterials and photonic crystals have shown negative refraction and subwavelength imaging at microwave and infrared frequencies. As discussed by Pendry [81], silver is a candidate for optical superlensing. Recently, Zhang et al. have demonstrated optical imaging with a silver superlens [128]. They showed sub-diffraction limited imaging with a resolution of one-sixth of the illumination wavelength (ultraviolet light at a 365 nm wavelength). This achievement is a result of their profound theoretical and experimental studies of the regeneration of evanescent waves by a silver film [129–131].

3.3 Photonic crystals

3.3.1 Realization

Photonic crystals are made of periodically modulated dielectric materials with a periodicity of the order of the wavelength of the electromagnetic wave. The resultant photonic dispersion exhibits a band nature analogous to the electronic band structure in a solid. When passing through photonic crystals, the propagation of electromagnetic waves can be significantly affected by the photonic crystals in the same way as the electrons are controlled by the crystals. Since their discovery in 1987 [4, 132], photonic crystals received a rapidly growing attention. The idea of controlling the light by means of photonic crystals has lead to many proposals for novel devices [2, 7–12].

Considerable efforts have been made to find photonic crystals that can completely block propagation of electromagnetic waves in all directions and for all polarizations within a certain frequency range, known as the photonic band gap. In the last two decades several three-dimensional photonic crystal architectures have been proposed and/or produced for this purpose. Among them are the criss-crossing pore structures (inverse diamond lattice of overlapping air spheres in a high dielectric background) [4, 133], slanted-pore structures [134], the woodpile structures [135, 136], inverse opal structures [137, 138], circular spiral structures [139], structures from woven dielectric fibers [140], square spiral structures [141–143], self-assemblies of metal nanospheres [144, 145], and bicontinuous and multicontinuous cubic microstructures [146–151]. The nanofabrication technology needed for their realization at optical and near infrared frequencies include angle etching [152–154], colloidal precipitation [155, 156], photopolymerization [157, 159], layer-by-layer [135, 160–165], and microassembly [166, 167] methods. An overview of the methods employed to obtain one-, two-, and three-dimensional photonic crystals mainly functioning in the optical range, is for example given in [12].
3. Light propagation in dielectric materials

3.3.2 Negative effective refractive index

Photonic crystals are not only of interest for applications related to their photonic band gap or to the possibility to localize modes around defects in the photonic crystal lattice. They also show other intriguing optical phenomena, such as superprism, negative refraction or ultra-reflective phenomena [3, 5, 6, 17, 168, 169]. The dielectric properties of photonic crystals, which are composite systems of constituents with different optical properties, are inhomogeneous. However, Notomi has shown that near the photonic band gap frequency, photonic crystals behave as if they have a certain effective refractive index which is not limited by the refractive index of the constituents but is determined by the photonic band structure [3, 17]. The effective refractive index can be smaller than one and can also be negative without absorption [3, 17]. As a result photonic crystals can be used to realize artificial dielectric materials having a negative refractive index.

The occurrence of negative refraction due to a negative index in two-dimensional photonic crystals consisting of dielectric rods arranged in a triangular lattice has been demonstrated by various numerical simulations [3, 17, 65, 79, 170] and has also been experimentally verified in the microwave regime [116]. The latter experiment has been criticized by Ye [66] since the authors did not verify the isotropy before applying Snell’s law. Moreover, the simulation results presented in Fig. 3 of [116], that are said to be in good agreement with the experimental results, show that inside the prism the light beam is not propagating along a straight line as expected for an (effective) isotropic medium. Experimental and theoretical evidence for focusing in a two-dimensional photonic crystal consisting of a triangular lattice of alumina rods in air is given in [120, 121, 124]. Focusing in a two-dimensional photonic crystal consisting of a triangular lattice of air holes drilled in a dielectric slab has also been numerically demonstrated and analyzed in detail [171-175] and observed experimentally for wavelengths in the infrared [119] and microwave [118] regime. However, the simulation results in [171] do not show focusing of the light inside the photonic crystal slab, as required for a negative index lens. Apart from negative refraction and imaging by a flat lens, another phenomenon relying on the concept of a negative refractive index has been simulated using photonic crystals with triangular lattice symmetry, namely open cavity formation [176-178].

It has also been shown theoretically that several photonic configurations consisting of air holes or dielectric rods in a square lattice can exhibit similar optical phenomena as the ones predicted for negative index materials, including negative refraction and imaging by a planar interface [179] and backward Cerenkov radiation [180], although the refraction index is anisotropic and positive. However, the latter type of imaging has been subject of debate. Li and Lin concluded that in this case the imaging properties are dominantly governed by the self-collimation effect and complex near-field scattering effects and not by the all-angle negative-refraction [181]. On the other hand it was shown by He et al. [182] that the negative refraction gives an important contribution to the focusing properties. They found that the
self-collimation effect occurs for small angles of incidence whereas the negative refraction effect occurs for relatively large angles of incidence [182]. As well in [181] as in [182] it was demonstrated that in the photonic crystals with square lattice symmetry no flat slab lensing, as described in Section 3.2.4 occurs. Namely, the slab-image distance dependency on the slab thickness is not observed [181, 182]. Furthermore, no focusing of the light inside the photonic crystal slab was found [181]. Based on an extensive simulation study Ye and co-workers concluded that the imaging properties are due to guided or collimated wave transmission caused by the presence of a partial band gap and not by negative refraction [66, 183–187].

The focusing of light with two-dimensional photonic crystals consisting of rods arranged in a square lattice has been demonstrated experimentally operating in the microwave regime [113–115]. However, Kuo and Ye found that the focusing reported in [115] is due to anisotropic scattering of the array of rods [66, 188]. Also the experiment of Cubukcu et al. [114] has been criticized [66] since the medium is not isotropic and then Snell’s law cannot be applied. Moreover, recently it has been shown that the so-called images of two point sources in [114], that are separated by a distance of $\lambda/3$, are due to the anisotropic scattering in the photonic crystal slab and due to the concentration of light in two of the rods at the exit interface [189]. The intensity distribution in a detection plane, placed close to the exit surface of the photonic crystal slab, depends on the light distribution concentrated in the cylinders at the exit interface [189]. As a result, “imaging” disappears if the distance between the sources is varied and if the sources are placed further away from the photonic crystal slab [189]. In both cases a larger number of cylinders light up at the exit plane and no images can be observed in the detection plane.

Recently, three-dimensional subwavelength imaging by a photonic-crystal flat lens using negative refraction at microwave frequencies has been demonstrated experimentally [127], a few years after the theoretical proposal of such lenses in [125, 126]. The photonic crystal used in the experiment is a BCC structure, similar as the one proposed by Luo et al. [125]. Within a certain frequency, negative refraction due to a negative effective refraction index, can be observed in this three-dimensional photonic crystal. In the experiment, imaging of a point source is demonstrated in both amplitude and phase [125]. Further validation of the subwavelength imaging is given by the imaging of two pinhole sources with subwavelength spacing as two resolvable spots.

### 3.3.3 Bloch waves

In the rest of this and the following chapters, we consider two-dimensional photonic crystals. The photonic crystal structure consists of a two-dimensional lattice of either dielectric cylinders with permittivity $\varepsilon$ embedded in air or air holes embedded in a dielectric medium with permittivity $\varepsilon$. The dielectric materials are assumed to be non-magnetic and therefore
\( \mu = 1 \). We only consider square and triangular lattices. We denote the primitive vector of the direct lattice by \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \) and the primitive vector of the reciprocal lattice by \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \) (see Appendix [A]).

Since the permittivity is a periodic function following the same periodicity as the photonic crystal lattice,

\[
\varepsilon(\mathbf{r} + \mathbf{R}) = \varepsilon(\mathbf{r}),
\]

for all \( \mathbf{R} \) in the Bravais lattice, we can write

\[
\varepsilon(\mathbf{r}) = \sum_{\mathbf{K}} \tilde{\varepsilon}(\mathbf{K}) e^{i\mathbf{K} \cdot \mathbf{r}},
\]

where \( \tilde{\varepsilon}(\mathbf{K}) \) are the Fourier coefficients of the function \( \varepsilon(\mathbf{r}) \) and \( \mathbf{K} \) are the reciprocal lattice vectors.

Using the notation

\[
\mathbf{K} = l\mathbf{b}_1 + m\mathbf{b}_2 \equiv \mathbf{K}_{l,m},
\]

Eq. (3.68) can be rewritten as

\[
\varepsilon(\mathbf{r}) = \sum_{l,m} \tilde{\varepsilon}(\mathbf{K}_{l,m}) e^{i\mathbf{K}_{l,m} \cdot \mathbf{r}},
\]

For later use, we define

\[
\varepsilon(\mathbf{r})^{-1} = \sum_{l,m} \hat{\varepsilon}(\mathbf{K}_{l,m}) e^{i\mathbf{K}_{l,m} \cdot \mathbf{r}},
\]

since the inverse of a periodic function is periodic itself. Here \( \hat{\varepsilon}(\mathbf{K}_{l,m}) \) denote the Fourier coefficients of the function \( \varepsilon(\mathbf{r})^{-1} \).

The electromagnetic wave that propagates in a photonic crystal is a Bloch wave. A Bloch wave can be written as

\[
\mathbf{V}(\mathbf{r}, t) = e^{-i(\omega_{n,k} - \mathbf{k} \cdot \mathbf{r})} \mathbf{u}_{n,k}(\mathbf{r}),
\]

where \( \mathbf{k} \) is the wave vector of the Bloch wave, \( \omega_{n,k} \) denotes the frequency in band \( n \) corresponding to \( k \) (see below for an explanation of the band index \( n \)) and \( \mathbf{u}_{n,k}(\mathbf{r}) \) is a periodic function having the same periodicity as the photonic crystal lattice:

\[
\mathbf{u}_{n,k}(\mathbf{r} + \mathbf{R}) = \mathbf{u}_{n,k}(\mathbf{r}),
\]

for all \( \mathbf{R} \) in the Bravais lattice. From Eq. (3.72) and Eq. (3.73) it follows that

\[
\mathbf{V}(\mathbf{r} + \mathbf{R}, t) = e^{i\mathbf{K} \cdot \mathbf{R}} \mathbf{V}(\mathbf{r}, t).
\]
Since a periodic function can always be expanded as a Fourier series, we can write

$$u_{n,k}(r) = \sum_{l,m} \tilde{u}_{n,k}(K_{l,m}) e^{iK_{l,m} \cdot r},$$  \hspace{1cm} (3.75)

where $\tilde{u}_{n,k}(K_{l,m})$ are the Fourier coefficients of $u_{n,k}(r)$. Substituting Eq. (3.75) in the Bloch theorem, Eq. (3.72), gives

$$V(r,t) = \sum_{l,m} \tilde{u}_{n,k}(K_{l,m}) e^{-i(\omega_{n,k} t - k_{l,m} \cdot r)},$$  \hspace{1cm} (3.76)

where we used the notation

$$k_{l,m} \equiv k + K_{l,m}.$$  \hspace{1cm} (3.77)

Expression (3.76) holds for the field vector $E$ and $H$. Hence, we can write

$$E(r,t) = \sum_{l,m} \tilde{E}_{n,k}(K_{l,m}) e^{-i(\omega_{n,k} t - k_{l,m} \cdot r)},$$  \hspace{1cm} (3.78a)

$$H(r,t) = \sum_{l,m} \tilde{H}_{n,k}(K_{l,m}) e^{-i(\omega_{n,k} t - k_{l,m} \cdot r)}.$$  \hspace{1cm} (3.78b)

### 3.3.4 Photonic band structure diagram

Substituting Eq. (3.78) with $\mu = 1$ and $M(t) = 0$ in Eq. (2.4a) gives

$$\sum_{l,m} [k_{l,m} \times \tilde{E}_{n,k}(K_{l,m}) - \omega_{n,k} \tilde{H}_{n,k}(K_{l,m})] e^{-i(\omega_{n,k} t - k_{l,m} \cdot r)} = 0.$$  \hspace{1cm} (3.79)

Since the plane waves satisfying the boundary condition

$$V(r + R, t) = V(r, t),$$  \hspace{1cm} (3.80)

with $R$ a general Bravais lattice vector, are an orthogonal set, the coefficient of each separate term in Eq. (3.79) must vanish, and therefore for all allowed wave vectors $k_{l,m}$

$$\tilde{H}_{n,k}(K_{l,m}) = \frac{1}{\omega_{n,k}} k_{l,m} \times \tilde{E}_{n,k}(K_{l,m}).$$  \hspace{1cm} (3.81)

Substituting Eq. (3.71) and Eq. (3.78) with $J(t) = 0$ in Eq. (2.4b) gives another relation between the Fourier coefficients of the fields

$$\tilde{E}_{n,k}(K_{l,m}) = - \frac{1}{\omega} \sum_{l',m'} \varepsilon(K_{l-l',m-m'}) k_{l',m'} \times \tilde{H}_{n,k}(K_{l',m'}).$$  \hspace{1cm} (3.82)
As seen in Chapter 2, in two-dimensional the time-dependent Maxwell equations separate into two sets of equations, one set for the TM polarization and one set for the TE polarization. For the TM mode we have

\[ \mathbf{\hat{H}}_{k,n} = (\hat{H}^x_{k,n}, \hat{H}^y_{k,n}, 0), \quad \mathbf{\hat{E}}_{k,n} = (0, 0, \hat{E}^z_{k,n}). \] (3.83)

Since in two-dimensional

\[ \mathbf{k}_{l,m} = (k^x_{l,m}, k^y_{l,m}, 0), \] (3.84)

we also have

\[ \mathbf{k}_{l,m} \cdot \mathbf{\hat{E}}_{k,n} = 0. \] (3.85)

Substituting Eq. (3.81) in Eq. (3.82) and making use of Eq. (3.83) and Eq. (3.85) leads to

\[ \omega^2 n, k \mathbf{\hat{E}}_{k,n}(\mathbf{K}_{l,m}) = \sum_{l',m'} \hat{\varepsilon}(\mathbf{K}_{l-l',m-m'}) |\mathbf{k}_{l',m'}|^2 \mathbf{\hat{E}}_{k,n}(\mathbf{K}_{l',m'}). \] (3.86)

The (infinitely many) different solutions to Eq. (3.86) for a given \( k \) are labeled with the band index \( n \). For \( |l|, |m| \leq N \), with \( N \) an arbitrarily large integer, Eq. (3.86) is the standard eigenvalue expansion used in the plane wave expansion method to compute the photonic band structure diagram of TM polarized waves in two-dimensional photonic crystals [2, 18, 190]. The wave vector \( k \) can be chosen to be in the first Brillouin zone, but this is not required. A wave vector \( k \) that does not lie in the first Brillouin zone can be written as \( k = k' - \mathbf{K} \) where \( k' \) lies in the first Brillouin zone (see Appendix A). If we draw the dispersion curve for all possible \( k \) vectors, then we use a representation known as the extended-zone scheme [191]. If we specify all the frequencies by a wave vector \( k \) in the first Brillouin zone, then we must fold all the bands displayed in the extended zone scheme in the first Brillouin zone by translation through reciprocal lattice vectors. This representation is known as the reduced zone scheme [191]. The representation in the reduced scheme can be periodically extended throughout all the \( k \)-space. This representation is called the repeated zone scheme [191].

For the TE mode, for which we have

\[ \mathbf{\hat{H}}_{k,n} = (0, 0, \hat{H}^x_{k,n}), \quad \mathbf{\hat{E}}_{k,n} = (\hat{E}^x_{k,n}, \hat{E}^y_{k,n}, 0), \] (3.87)

the photonic band structure diagram can be calculated as follows. Substituting Eq. (3.82) in Eq. (3.81) and making use of Eq. (3.87) and of

\[ \mathbf{k}_{l,m} \cdot \mathbf{H}_{k,n} = 0, \] (3.88)
yields
\[ \omega_n^2 \hat{H}_k^{z,l,m}(K_{l,m}) = \sum_{l',m'} \hat{\varepsilon}(K_{l-l',m-m'}) \hat{H}_k^{z,l,m}(K_{l',m'}) (k \cdot k_{l,m}'). \] (3.89)

As for the TM case, Eq. (3.89) with \(|l|, |m| \leq N\) allows to compute the photonic band structure diagram of TE polarized waves in two-dimensional photonic crystals.

From the photonic band structure diagram, the equifrequency surfaces (EFSs), that are surfaces of equal frequency in \(k\) space, can be obtained for the various photonic bands. Note that although in two dimensions we rather have equifrequency contours instead of EFS, in what follows we always use the term EFS. Since the photonic band structure diagram can be displayed in the reduced, repeated and extended zone scheme, also the EFSs can be displayed in these three schemes.

### 3.3.5 Wave vector diagram

In conventional geometrical optics, light propagation in dielectric materials is described by the phase refractive index and Snell’s law (see Section 3.1). Light propagation in periodic structures, of which photonic crystals are an example, is different from that in conventional materials. The refraction phenomenon relies on the conservation of the wave vector and due to the periodical nature of these structures the wave vector \( k \) is not conserved. The direction of light propagation inside a photonic crystal is determined by the EFSs [3, 17, 192]. Notomi [3, 17] has theoretically analyzed the light propagation phenomenon in periodic structures and photonic crystals with the help of the band structure theory and numerical simulations. A more recent detailed systematic study of refraction phenomena occurring in two-dimensional photonic crystals based on the wave vector diagram formalism can be found in [18]. In this section we closely follow [3, 17, 18] to explain the wave vector diagram analysis.

We first consider a very simple example of wave vector diagram analysis shown in Fig. 3.11a, which graphically describes a light incident problem from air to a dielectric material. The wave vector diagram contains the EFSs that apply for the frequency of operation. For any isotropic homogeneous material, the EFS is a circle with radius \( k = |k| = |n| \omega/c \), \( k \) being the wave vector, \(|n|\) the refractive index of the medium, \( \omega \) the working frequency, and \( c \) the velocity of light in vacuum. For conventional isotropic homogeneous dielectric materials the phase refractive index is always larger than one. Hence, the circle for the dielectric material in Fig. 3.11a is larger than the one for air which has a refractive index equal to one. The incoming wave vector \( k \) is drawn on the reciprocal lattice such that it starts at the origin of the reciprocal lattice and such that it points in the direction of the incident wave. The length of \( k \) is determined by the EFS contour in air.
Figure 3.11: Wave vector diagram for a light incident problem from air \((n = 1)\) to a homogeneous isotropic dielectric material with refractive index \(\hat{n} > 1\) (a) and from air \((n = 1)\) to a photonic crystal with \(\hat{n} < 0\) (b). \(k\) and \(\hat{k}\) denote the incident and refracted wave vector, respectively; \(v_g\) and \(\hat{v}_g\) denote the corresponding group velocity vectors.

The tangential components of the wave vector \(k\) are always conserved at an interface between two isotropic materials. The \(k_{\parallel}\) conservation condition, indicated by the dotted line in Fig. 3.11a, determines the allowed refracted wave vectors \(\hat{k}\). There are two choices for \(\hat{k}\) (to point either towards A or towards B). The propagation direction is determined by the group velocity \(\hat{v}_g = \nabla_{\hat{k}} \omega\) which is perpendicular to the EFS at the allowed \(\hat{k}\) points (point A or B) and which points towards increasing values of frequency. Since for a conventional homogeneous isotropic dielectric medium \(n\) is always larger than one, the radii of the EFS increase with increasing frequency. Hence the group velocity always points outwards and \(\hat{v}_g \cdot \hat{k} > 0\). Furthermore, the correct choice of \(\hat{k}\) is the one that gives a \(\hat{v}_g\) that points away from the source. Hence, in this case \(\hat{k}\) should point to B. In fact, Fig. 3.11a is simply a graphical representation of Snell’s law in \(k\) space \([3, 17]\)

\[
n_1 \sin \theta_1 = n_2 \sin \theta_2, \tag{3.90}
\]

where \(n_1\) and \(n_2\) are the phase refractive indices of material 1 and 2, respectively and \(\theta_1\) and \(\theta_2\) are the angles the propagation directions in material 1 and 2 make with respect to the interface normal (see Fig. 3.1).

A similar graphical picture can be made to study light propagation in diffraction gratings and photonic crystals \([3, 17, 68, 79, 168, 170, 179, 193, 196]\). For these structures, the EFSs are periodically repeated in the wave vector diagram and the \(k_{\parallel}\) conservation rule is generalized.
3.3. Photonic crystals

to satisfy the periodic boundary condition. The $k_\parallel$ conservation condition reads

$$k_\parallel, m = k \sin \theta + \frac{2\pi m}{a_s},$$ (3.91)

where $k$ denotes the length of the incoming wave vector, $\theta$ denotes the angle of incidence, $a_s$ represents the periodicity of the interface and $m$ is an integer equal to 0, ±1, ±2, . . . . In the wave vector diagram, Eq. (3.91) is represented by $m$ parallel lines, all perpendicular to the interface and separated by a distance $2\pi m/a_s$. The lines are often called construction lines \[194\. Using the vector diagram analysis, Notomi has shown that the propagation characteristics of diffraction gratings and weakly modulated photonic crystals, that is photonic crystals built from constituents with a small difference in dielectric constant ($\mu = 1$), are very similar \[3, 17\. For such periodic structures a phase index in terms of Snell’s law cannot be defined \[3, 17\. If one would define a phase index, the index would strongly depend on the incident angle and therefore Snell’s law loses its meaning. However, the wave vector diagram analysis can be used to explain typical features of a diffraction grating such as, for example, beam decomposition into diffracted waves and strong sensitivity of beam propagation to the incident angle and wavelength \[3, 17\. Also the anomalous light propagation reported for photonic crystals such as for example the superprism effect and the ultrarefractive properties can be understood within this picture \[3, 17\. Thus these phenomena cannot be understood within a refraction picture and must be understood as diffraction. Note that for a complete understanding of light propagation in diffraction gratings and photonic crystals it is not sufficient to study propagation modes in the first Brillouin zone \[3, 18\. All allowed propagation modes in the repeated zone scheme should be investigated \[3, 18\. However for strongly modulated photonic crystals near the photonic band gap an effective phase refractive index can be defined to explain the light propagation inside the photonic crystal using Snell’s law and this in spite of the presence of strong multiple diffraction \[3, 17\. For simplicity of notation, we also denote this effective refractive index by $n$. In strongly modulated photonic crystals, the phase refractive index can be smaller than one and can also be negative. This can lead to unusual refraction phenomena such as ultrarefractivity and negative refraction.

To explain this we consider a two-dimensional photonic crystal slab made from dielectric pillars with radius $r = 0.35a$ and $\tilde{n} = 3.6$ arranged in a triangular lattice with lattice constant $a$ \[3, 17\. We use the MIT Photonic-Bands software \[190\. to calculate the photonic band structure diagram for the TE-mode. The result is shown in Fig. 3.12. For the dimensionless frequency range $f = \omega a/2\pi c \in [0.562, 0.607]$, we obtain the EFS depicted in Fig. 3.13. From Fig. 3.13 it can be seen that for increasing frequencies, that is for frequencies coming close to one of the gap frequencies, the shape of the EFSs becomes rounded and finally becomes circular. In the latter case, the EFS plot looks similar to that of a conventional dielectric material as shown in Fig. 3.11. This means that we can define an effective refractive
index  \( \hat{n} \) from the radius of the EFS using Snell’s law, suggesting that for these frequencies the beam propagation is refraction like. However, for these frequencies there is a striking difference from conventional refraction. For example, for the frequency \( f = 0.6 \), the radius of the EFS gives \( |\hat{n}| = 0.47 \). Hence, in the schematic picture that describes the light incident problem from air to the photonic crystal, the circle (equifrequency contour) for air is larger than the one for the photonic crystal (see Fig. 3.11b). As a consequence, for certain angles of incidence no light beam propagates in the photonic crystal since the light is totally reflected off the interface. This corresponds to total internal reflection, a phenomenon which does not occur when a light beam is incident from air to a conventional material.

The sign of \( \hat{n} \) is determined from the behavior of the EFSs. In this case the EFSs move inwards with increasing frequency, as can be seen from Fig. 3.13. Hence \( \hat{\nu}_g \cdot \hat{k} < 0 \). It can be proven analytically that for the infinite photonic crystal system, the direction of the group velocity coincides with the direction of the energy velocity \([58][197]\). Therefore, the group velocity vector represents the direction of propagation for the electromagnetic wave in the photonic crystal. The sign of \( \hat{n} \) is given by the sign of \( \hat{\nu}_g \cdot \hat{k} \) (see Section 3.2.1). Thus in this
3.3. Photonic crystals

Figure 3.13: EFS plot of TE modes in a two-dimensional photonic crystal made from dielectric pillars with radius \( r = 0.35a \) and refractive index \( \hat{n} = 3.6 \) positioned in a triangular lattice with lattice constant \( a \). The frequencies \( f \) range from 0.562 to 0.607. The first Brillouin zone of a triangular lattice (dotted line) and the symmetry points are also shown (see Appendix A).

In this case we have \( \hat{n} = -0.47 \). The propagation direction of the electromagnetic wave is inward. This results in a negative propagation angle for all incident angles. Schematically, this can be seen from Fig. 3.11b. Due to the \( k_\parallel \) conservation rule, there are two choices for \( k \), to point towards A or to point towards B. Since the direction of propagation is determined by the group velocity and points away from the source, \( k \) should point to A. The group velocity is perpendicular to the EFS at point A. Note that for this particular example, it is sufficient to study the propagation modes in the first Brillouin zone only. Therefore it is sufficient to display the EFSs in the reduced zone scheme. In what follows, we will only use the extended or repeated zone scheme if it is necessary to explain the wave propagation.

The wave vector diagram analysis method is an adequate method to determine the propagation angles. However, since the method gives no information on the amplitude across the interface, it cannot be predicted whether or not waves with these propagation angles are excited by the incident wave.
3. Light propagation in dielectric materials

3.3.6 Note on the use of two-dimensional models

Since three-dimensional FDTD calculations are very time and computer memory consuming and since we want to explore a large parameter space we study in the following chapters only three-dimensional photonic crystals with translational invariance in the \( z \)-direction. As mentioned before, in this case the numerical problem of solving the time-dependent Maxwell equations reduces to a two-dimensional problem and the time-dependent Maxwell equations can be solved for the TM and TE mode separately.

In contrast to these pure two-dimensional photonic crystals, the two-dimensional photonic crystals investigated in many experiments are not infinite in the \( z \)-direction. Two-dimensional photonic crystals are often fabricated by sandwiching a central layer of a dielectric material between two other layers with a lower index of refraction than the central layer. Note that the two outer layers can also be considered to be air so that only one thin layer of dielectric material is present. The upper and lower layer can be chosen to be identical in order to construct a so-called symmetric waveguide, or different, to construct an asymmetric waveguide.

In most cases the photonic crystals consist of a periodic pattern of air holes deeply etched in these waveguide structures, but several other constructions can be thought of \[198\]. All these structures are called planar photonic crystals or photonic crystal slabs. We prefer the name planar photonic crystals in order to make a distinction between slabs in two and three dimensions. Namely, a two-dimensional plate of a photonic crystal is also called a slab. In what follows, we only consider symmetric waveguides.

In planar photonic crystals, electromagnetic waves are confined in the vertical direction by waveguiding with dielectric index mismatch and in the horizontal direction by the two-dimensional photonic crystal. Two-dimensional calculations cannot be used to study these three-dimensional structures. However, in order to minimize the computational efforts, the theoretical analysis of these structures is often restricted to two-dimensional approximate models, making use of an effective refractive index \[199, 200\]. In order to identify the modes that can radiate vertically, the projected band structure is computed. The eigensolutions of the bulk top and bottom layer are \( \omega = c \sqrt{|k|^2 + k_z^2/n_0} \), where \( n_0 \) denotes the refractive index of the dielectric material of the top and bottom layer, \( k = (k_x, k_y) \) denotes the two-dimensional Bloch wave vector and \( k_z \) denotes the \( z \)-component (vertical component) of the wave vector. If these eigensolutions are plotted against \( k \), they form the so-called light cone \( \omega \geq c |k|/n_0 \).

The light-line \( \omega = c |k|/n_0 \) in the photonic band structure diagram separates the radiation from the guided modes. The guided modes lie below the light line and are stationary Bloch modes that are ideally not subject to propagation losses. These modes are infinitely extended within the plane of the planar photonic crystal and decay exponentially into the vertical direction. This confinement is analogous to internal reflection and is due to the difference in refractive index between the central and outer layers (higher effective refractive index in the central layer compared to the refractive index in the outer layers). Above the light line, the
Photonic crystals spectrum becomes a continuum of modes. At the edge of the light cone, there exist resonances called quasi-guided modes. These modes exhibit intrinsic propagation losses due to out-of-plane diffraction. Photonic band gaps that are complete for a pure two-dimensional photonic crystal become incomplete band gaps in the guided mode spectrum. For a planar two-dimensional photonic crystal, a band gap is a range of frequencies in which no guided modes exist. It is an incomplete band gap because there are still radiation modes at those frequencies. The presence of a gap is strongly dependent on the thickness of the planar photonic crystal [198]. The height of the planar photonic crystal should not be too small in order not to have a weak confinement of the modes inside the structure and not too large in order not to allow higher order modes that fill the gap. If, as in the cases we consider in this section, the horizontal mid-plane of the planar photonic crystal is a mirror symmetry plane, then the guided bands can be classified according to whether they are even or odd with respect to reflections through this plane. These even and odd modes have strong similarities with the TE and TM modes, respectively, of the ideal two-dimensional photonic crystal, and are therefore called TE-like and TM-like modes. Note that in the mirror plane itself, the even and odd modes are pure TE and TM modes, respectively.

Comparison of approximate two-dimensional calculations that use an effective refractive index with full three-dimensional calculations has shown that good qualitative agreement can be obtained [199, 200]. Evidently, the two-dimensional transmission is considerably larger than the corresponding three-dimensional transmission because no out-of-plane losses are included in the two-dimensional calculations [200]. In [201], a two-dimensional study of losses in planar photonic crystals has been made using a two-dimensional model, which treats a system of trenches etched in the step-index dielectric waveguide [201]. Also in this study good qualitative agreement has been found with the full three-dimensional results [201]. Hence, two-dimensional numerical studies can provide sufficient guidance in designing planar photonic crystals for various purposes.

In the following chapters we consider pure two-dimensional photonic crystals and not the planar photonic crystals as mentioned before. However, these planar photonic crystals are only one alternative to real three-dimensional photonic crystals studied in experiments. Namely, in order to have, in experiments, full control of electromagnetic wave propagation in photonic crystals, a complete photonic band gap is required. This can only be found in a three-dimensional photonic crystal, but they are very difficult to fabricate (see Section 3.3.1). As an alternative, three-dimensional crystals are made from their two-dimensional analogues, either by making planar photonic crystals, having vertical radiation losses that can be minimized to tolerable levels by various strategies, or by making photonic crystals with very deep holes or very long cylinders, that is by increasing the vertical dimension of the photonic crystal until this dimension can be treated as infinite. Macroporous silicon is an example of the latter kind of photonic crystals [202–205]. Recently, a similar photonic crystal made from another material was used to demonstrate negative refraction and to make a lens with subwavelength...
resolution [118]. Our two-dimensional simulation results presented in the following chapters can provide guidance in designing these very long hole or very long cylinders type of photonic crystals for various purposes.