Why history matters: \textit{ab initio} rederivation of Fresnel equations confirms microscopic theory of refractive index

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Abstract

We provide a systematic theoretical, experimental, and historical critique of the standard derivation of Fresnel’s equations, which shows in particular that these well-established equations actually contradict the traditional, macroscopic approach to electrodynamics in media. Subsequently, we give a rederivation of Fresnel’s equations which is exclusively based on the microscopic Maxwell equations and hence in accordance with modern first-principles materials physics. In particular, as a main outcome of this analysis being of a more general interest, we propose the most general boundary conditions on electric and magnetic fields which are valid on the microscopic level.

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1. Introduction

Introduced by P. Nozières and D. Pines in 1958 as the “generalized dielectric constant at arbitrary frequency \( \omega \) and wavevector \( k \) [1, p. 470, notation adapted], the dielectric function soon turned into a concept of outstanding importance for ab initio materials physics. On the theoretical side, it had already been instrumental for the very development of first-principles methods [2–6], only to become itself a prime target quantity for both Green function theory and density functional theory (see e.g. Refs. [7–9] for classical reviews). Practically, knowledge of the dielectric function does not only allow one to access—via the zero-frequency limit—the age-old dielectric constant, but also the optical conductivity, the density response function, and finally—via the famous Maxwell relation—even the refractive index and its ensuing optical properties such as the reflectance. At present, the prediction of the dielectric function therefore ranks among the most active areas in both experimental and theoretical research (see Refs. [10–20] for recent examples).

However, as has become clear since the advent of the Modern Theory of Polarization [21–23], current first-principles methods (see e.g. Refs. [24–30] for modern textbooks) used to access the dielectric function differ profoundly from their traditional counterparts. While the latter had been formulated macroscopically in terms of “dipole densities”, ab initio methods rely on a microscopic formulation in terms of “external” and “induced” electromagnetic fields. In fact, this provides a new framework of electrodynamics in media, which is in stark contrast to most traditional textbooks (see e.g. Refs. [31, §7.3] or [32, §9.3.3]). Recently, the authors of this article have therefore condensed the corresponding common practice of ab initio materials physics into the Functional Approach to electrodynamics of media [34–41], which is an inherently microscopic theory of electromagnetic material properties. With these developments, however, the following fundamental problem arises: the classical methods for the measurement of the dielectric function, such as ellipsometry or reflectivity spectroscopy (see e.g. Ref. [42, §6.1.2]), rely on Fresnel’s equations, and these are usually derived in the phenomenological framework of macroscopic electrodynamics (see e.g. Refs. [31, §7.3] or [32, §9.3.3]). It therefore remains to prove that Fresnel’s equations can also be justified within the microscopic framework which is actually used for the calculation of the dielectric function from first principles. This is precisely the main objective of the present article.

Concretely, we address this problem as follows. After a short introduction
to Fresnel’s equations in Sct. 2 and a review of their standard derivation in § 3.1, we proceed in § 3.2 with a historical review of the experimental and theoretical developments which eventually led to this standard derivation. With this, we go on to subject the standard derivation of Fresnel’s equations to a thorough critique (§ 3.3). Finally, in Sct. 4 we discuss the problem of general electromagnetic boundary conditions on the microscopic level, and we present a completely microscopic derivation of Fresnel’s equations.

2. Fresnel equations and optical properties

We consider an ordinary refraction experiment with an incident light ray impinging on the flat interface between two materials with refractive indices $n_1$ and $n_2$. In most cases, the incident ray will be split into a reflected part and a transmitted (or refracted) part, whose directions are given in terms of the respective refractive indices by the law of reflection,

$$\varphi_r = \varphi_1,$$  \hspace{1cm} (2.1)

and by Snellius’ law of refraction,

$$n_1 \sin \varphi_1 = n_2 \sin \varphi_2.$$  \hspace{1cm} (2.2)

Here, $\varphi_1$ is the angle of incidence measured with respect to the surface normal, while $\varphi_r$ and $\varphi_2$ are the respective angles of the reflected and the refracted light rays. In this situation, the Fresnel equations determine the polarization-dependent electric field amplitudes of the reflected and the transmitted rays relative to the field amplitude of the incident ray. Concretely, Fresnel’s equations read as follows (see, for example, Ref. [43, Eqs. (4.270)–(4.273)]):

$$\left( \frac{E_r}{E_i} \right)_s = \frac{2n_1 \cos \varphi_1}{n_1 \cos \varphi_1 + n_2 \cos \varphi_2},$$  \hspace{1cm} (2.3)

$$\left( \frac{E_r}{E_i} \right)_p = \frac{n_1 \cos \varphi_1 - n_2 \cos \varphi_2}{n_1 \cos \varphi_1 + n_2 \cos \varphi_2},$$  \hspace{1cm} (2.4)

$$\left( \frac{E_t}{E_i} \right)_s = \frac{2n_1 \cos \varphi_1}{n_2 \cos \varphi_1 + n_1 \cos \varphi_2},$$  \hspace{1cm} (2.5)

$$\left( \frac{E_t}{E_i} \right)_p = \frac{n_2 \cos \varphi_1 - n_1 \cos \varphi_2}{n_2 \cos \varphi_1 + n_1 \cos \varphi_2}.$$  \hspace{1cm} (2.6)
Here, \( E_i \), \( E_r \) and \( E_t \) respectively denote the electric field amplitudes of the incident, reflected and transmitted (or refracted) light rays. Finally, the subscripts “s” and “p” refer to the polarization orthogonal (“senkrecht”) and parallel to the plane of incidence (which is defined by the direction of the incident ray and the surface normal). By invoking Snellius’ law of refraction, the above equations further simplify to \[43\] Eqs. (4.274)–(4.277)

\[
\left( \frac{E_t}{E_i} \right)_s = \frac{2 \cos \varphi_1 \sin \varphi_2}{\sin(\varphi_2 + \varphi_1)},
\] (2.7)

\[
\left( \frac{E_r}{E_i} \right)_s = \frac{\sin(\varphi_2 - \varphi_1)}{\sin(\varphi_2 + \varphi_1)},
\] (2.8)

\[
\left( \frac{E_t}{E_i} \right)_p = \frac{2 \cos \varphi_1 \sin \varphi_2}{\sin \varphi_1 \cos \varphi_1 + \sin \varphi_2 \cos \varphi_2},
\] (2.9)

\[
\left( \frac{E_r}{E_i} \right)_p = \frac{\tan(\varphi_1 - \varphi_2)}{\tan(\varphi_1 + \varphi_2)}.
\] (2.10)

These are in fact the original equations due to Augustin-Jean Fresnel (1788-1827). Correspondingly, Eqs. (2.8) and (2.10) are known as “Fresnel’s sine law” and “Fresnel’s tangent law”, respectively. Furthermore, the ratios \( r_s := (E_r/E_i)_s \) and \( r_p := (E_r/E_i)_p \) of the reflected field amplitudes to their incident counterpart are called reflectivities.

Apart from their outstanding theoretical value to be clarified below, the Fresnel equations are also of tremendous practical importance. Let us mention only the most important applications:

\( i \) \textbf{Brewster angle.} Setting Eq. (2.6) to zero leads to the condition

\[
n_2 \cos \varphi_1 = n_1 \cos \varphi_2.
\] (2.11)

Eliminating from this the variable \( \varphi_2 \) via the law of refraction, Eq. (2.2) we obtain after some algebra the equation \[43\ Eq. (4.278)]

\[
\tan \varphi_1 = \frac{n_2}{n_1},
\] (2.12)

which is the formula for the \textit{Brewster angle}. For light incident under this angle, the intensity of the reflected light with polarization parallel to the plane of incidence vanishes.
(ii) Reflectance. In vacuo, the ratio between incident and reflected intensities, i.e., the reflectance, is given by the squared modulus of the ratio between the corresponding field amplitudes (i.e., of the reflectivity). Concretely, considering normal incidence from the vacuum \((n_1 = 1)\), Snellius’ law implies that the angles of incidence and reflection are equal, hence \(\varphi_1 = \varphi_2 = 0\). With this, it is straightforward to show that the reflectance is independent of the polarization,

\[
R = |r_s|^2 = |r_p|^2,
\]

which is intuitive since for normal incidence the distinction between s- and p-polarization looses its meaning anyway. Furthermore, the reflectance is given by (see e.g. Refs. [42, Eq. (6.8)] or [44, Eq. (1.29)])

\[
R = \left| \frac{n_2 - 1}{n_2 + 1} \right|^2 = \frac{(\nu - 1)^2 + \kappa^2}{(\nu + 1)^2 + \kappa^2},
\]

where \(\nu := \Re n_2\) and \(\kappa := \Im n_2\) are the so-called optical constants, with \(\kappa\) being the extinction coefficient.

(iii) Ellipsometry. Finally, in ellipsometry experiments one considers again linearly polarized light incident from vacuum \((n_1 = 1)\) but at a non-zero angle \(\varphi_1\). In general, the reflected ray is then elliptically polarized, and from the Fresnel equations it can be shown directly that

\[
(\nu + i\kappa)^2 = \sin^2 \varphi_1 + \sin^2 \varphi_1 \tan^2 \varphi_1 \left( \frac{1 - r_p/r_s}{1 + r_p/r_s} \right)^2,
\]

from which the refractive index can be computed in terms of the reflectivities (see e.g. Ref. [42, Eq. (6.13)]). As the ratio of the reflectivities is a measurable quantity, Eq. (2.15) forms the basis of ellipsometric measurements of the dielectric function via the standard relation \(n^2 = \varepsilon_r\).

We note, in particular, that this would not be possible if the refractive index was given by the formula \(n^2 = \varepsilon_r \mu_r\).

Apart from ellipsometric measurements, Eqs. (2.12) and (2.14) are nowadays the basis for the deduction of the refractive index from the Brewster angle and from reflectivity spectra, respectively.
3. Standard Approach

3.1. Standard derivation of Fresnel equations

In the Standard Approach to electrodynamics in media, the Fresnel equations are derived from the so-called boundary conditions on the electromagnetic fields, which read (see e.g. Ref. [31, Eqs. (I.17)–(I.20)])

\begin{align*}
\mathbf{n} \cdot (\mathbf{D}_2 - \mathbf{D}_1) &= \rho_{\partial V}, \quad \text{(3.1)} \\
\mathbf{n} \times (\mathbf{E}_2 - \mathbf{E}_1) &= 0, \quad \text{(3.2)} \\
\mathbf{n} \cdot (\mathbf{B}_2 - \mathbf{B}_1) &= 0, \quad \text{(3.3)} \\
\mathbf{n} \times (\mathbf{H}_2 - \mathbf{H}_1) &= \mathbf{j}_{\partial V}, \quad \text{(3.4)}
\end{align*}

where \(\rho_{\partial V}\) and \(\mathbf{j}_{\partial V}\) are the surface charge and current densities, and \(\mathbf{n}\) denotes the surface normal pointing from material “1” to material “2”. To obtain the Fresnel equations, one then has to make three fundamental assumptions:

1. The incident, reflected and transmitted light rays are represented by transverse electromagnetic plane waves, with their corresponding wave-vectors being identical to the respective ray directions.

2. The surface currents and charges are set to zero:

\begin{align*}
\rho_{\partial V} &= 0, \quad \text{(3.5)} \\
\mathbf{j}_{\partial V} &= 0. \quad \text{(3.6)}
\end{align*}

3. The fields \(\mathbf{D}_j\) and \(\mathbf{H}_j\) are eliminated by the conventional material relations (for \(j = 1, 2\)),

\begin{align*}
\mathbf{D}_j &= \varepsilon_0 \varepsilon_{r,j} \mathbf{E}_j, \quad \text{(3.7)} \\
\mathbf{H}_j &= (\mu_0 \mu_{r,j})^{-1} \mathbf{B}_j, \quad \text{(3.8)}
\end{align*}

where the respective material parameters \(\varepsilon_{r,j}\) and \(\mu_{r,j}\) are assumed to be frequency-dependent constants.

In particular, the second and the third assumption together with Eqs. (3.1)–(3.4) imply the following boundary conditions for the electric field and the
magnetic field (see e.g. Ref. [31, Eqs. (7.37)]):
\[
\mathbf{n} \cdot (\varepsilon_{r,2} \mathbf{E}_2 - \varepsilon_{r,1} \mathbf{E}_1) = 0,
\]
(3.9)
\[
\mathbf{n} \times (\mathbf{E}_2 - \mathbf{E}_1) = 0
\]
(3.10)
\[
\mathbf{n} \cdot (\mathbf{B}_2 - \mathbf{B}_1) = 0
\]
(3.11)
\[
\mathbf{n} \times (\mathbf{B}_2/\mu_{r,2} - \mathbf{B}_1/\mu_{r,1}) = 0
\]
(3.12)

On account of the first assumption, one now starts from the following ansatz:
the respective light rays are given by the Fourier-mode contributions
\[
\mathbf{E}_i(x, t) = \mathbf{E}_{i,0} \exp(-i\omega_i t + i\mathbf{k}_i \cdot \mathbf{x}),
\]
(3.13)
\[
\mathbf{E}_r(x, t) = \mathbf{E}_{r,0} \exp(-i\omega_r t + i\mathbf{k}_r \cdot \mathbf{x}),
\]
(3.14)
\[
\mathbf{E}_t(x, t) = \mathbf{E}_{t,0} \exp(-i\omega_t t + i\mathbf{k}_t \cdot \mathbf{x}),
\]
(3.15)
where the plane waves are assumed to be transverse, i.e.,
\[
k_i \cdot \mathbf{E}_i = k_r \cdot \mathbf{E}_r = k_t \cdot \mathbf{E}_t = 0
\]
(3.16)
and the magnetic fields are related to the electric fields via Faraday’s law,
\[
\mathbf{B}_i = k_i \times \mathbf{E}_i/\omega_i,
\]
(3.17)
\[
\mathbf{B}_r = k_r \times \mathbf{E}_r/\omega_r,
\]
(3.18)
\[
\mathbf{B}_t = k_t \times \mathbf{E}_t/\omega_t.
\]
(3.19)

Furthermore, the frequencies are related to the wavevectors via the respective refractive indices, hence
\[
\frac{\omega_i}{c|\mathbf{k}_i|} = \frac{\omega_r}{c|\mathbf{k}_r|} = \frac{1}{n_1}, \quad \frac{\omega_t}{c|\mathbf{k}_t|} = \frac{1}{n_2}.
\]
(3.20)

Next, the amplitudes \( \mathbf{E}_{i,0}, \mathbf{E}_{r,0} \) and \( \mathbf{E}_{t,0} \) have to be chosen such that the electric and magnetic fields match the boundary conditions
(3.9)-(3.12) with
\[
\mathbf{E}_1 := \mathbf{E}_i + \mathbf{E}_r,
\]
(3.21)
\[
\mathbf{E}_2 := \mathbf{E}_t,
\]
(3.22)
and analogous equations for the magnetic fields. Independently of the polarization, these boundary conditions then imply the constancy of the frequency,
\[
\omega_i = \omega_r = \omega_t \equiv \omega,
\]
(3.23)
and moreover, they even re-imply the laws of reflection and refraction, which can then be condensed into (see Ref. [45, Eq. (4.6)])

$$n \times k_i = n \times k_t = n \times k_t.$$ (3.24)

Furthermore, for the ratios of the field amplitudes one finds after a more involved calculation (see Ref. [43, Eqs. (4.262), (4.264), (4.267) and (4.268)]):

$$\left( \frac{E_t}{E_i} \right)_s = \frac{2 Z_1^{-1} \cos \varphi_1}{Z_1^{-1} \cos \varphi_1 + Z_2^{-1} \cos \varphi_2},$$ (3.25)

$$\left( \frac{E_r}{E_i} \right)_s = \frac{Z_1^{-1} \cos \varphi_1 - Z_2^{-1} \cos \varphi_2}{Z_1^{-1} \cos \varphi_1 + Z_2^{-1} \cos \varphi_2},$$ (3.26)

$$\left( \frac{E_t}{E_i} \right)_p = \frac{2 Z_1^{-1} \cos \varphi_1}{Z_2^{-1} \cos \varphi_1 + Z_1^{-1} \cos \varphi_2},$$ (3.27)

$$\left( \frac{E_r}{E_i} \right)_p = \frac{Z_2^{-1} \cos \varphi_1 - Z_1^{-1} \cos \varphi_2}{Z_2^{-1} \cos \varphi_1 + Z_1^{-1} \cos \varphi_2},$$ (3.28)

where $E = |E|$, etc., and where $Z$ denotes the wave impedance defined for each material as

$$Z := \sqrt{\mu_r \varepsilon_r}.$$ (3.29)

Clearly, these formulae do not reproduce the Fresnel equations (2.3)–(2.6) if the refractive index is given by the standard formula

$$n \neq \sqrt{\varepsilon_r \mu_r}.$$ (3.30)

We will therefore refer to Eqs. (3.25)–(3.28) as the pseudo-Fresnel equations. In order to reproduce the real Fresnel formulae from these, one has to introduce the following additional assumption (see e.g. Ref. [31, §7.3]):

4. The relative permeabilities of both materials are equal to one, i.e.,

$$\mu_{r,1} = \mu_{r,2} = 1.$$ (3.31)

With this additional assumption, it follows that

$$n_j = \sqrt{\varepsilon_{r,j}},$$ (3.32)
and hence,
\[
\frac{1}{Z_j} = n_j.
\] (3.33)

In this case, Eqs. (3.25)-(3.28) imply the original Fresnel equations (2.3)-(2.6) and this completes their derivation in the Standard Approach.

3.2. Historical review

Both to put the above considerations into perspective and for the critique of the Standard Approach to be spelled out in the following subsection, we now provide a short historical account of the events that have finally led to the derivation of the Fresnel equations in the Standard Approach. We first summarize the developments in experimental physics up to the discovery of the Fresnel equations (§3.2.1), then shortly review the corresponding developments in theoretical physics (§3.2.2), and finally conclude with a comparative discussion of these events in §3.2.3. For short and readable introductions to the history of optics, the interested reader is referred to the respective chapters in Refs. [45–47], on which we have heavily drawn.

3.2.1. Experiment

Law of reflection.—Among all the facts adduced in the preceding subsections, only the law of reflection dates back to pre-modern times. In fact, this law had traditionally been ascribed to Euclid (ca. 365-300 BC), in whose Catoptrica it can be found (see Refs. [48, p. 10] or [49, p. 119]). Nowadays, however, this work is believed to be apocryphal (see ibid. or [50, p. 12]). In any case, the law of reflection was already known to the ancients as it can also be found in the works of Archimedes (ca. 287-212 BC), Hero (floruit ca. 60 AD), and Ptolemy (ca. 100-170 AD) [50, p. 13]. The fact that the incident and the reflected light rays lie in the same plane which also contains the surface normal has probably been known throughout all this time, but explicitly, it can at best be traced back to the important Arab scholar Ibn Al Haitam (also: Al Hazen; ca. 965-1040 AD) [48, pp. 21/22].

Law of refraction.—Compared to the law of reflection, the law of refraction is much younger, dating back to W. Snellius (1580 or 1591-1626) who discovered it in 1620 [51, p. 227]. The unpublished manuscript, however, is not extant. In its present form, the “law of sines” was given in 1637 by R. Descartes (1596-1650) in La Dioptrique [48, p. 83]. Already in 1665, it appeared in the monumental treatise De corpore of the English philosopher-physicist T. Hobbes (1588-1679). Not much later, namely in 1666, I. Newton
(1643-1727) discovered the phenomenon of dispersion, which implies that actually each wavelength has its own index of refraction (see Refs. [46, p. xxvi] or [52, p. 135]). Thus, around 1700 AD the most basic facts related to refraction and reflection independently of possible polarization effects were well-known to the scientific community.

Light polarization.—Although the polarization of light as such had already been described by C. Huygens (1629-1695) in 1690 [47, pp. 2/3], it was not until 1808/9 that E.-L. Malus (1775-1812) observed that reflected rays may be polarized [46, p. xxvii], [53, p. 37]. In 1816/9, D. F. J. Arago (1786-1853) together with the ingenious outsider A.-J. Fresnel (1788-1827) then proved that light rays polarized orthogonally to each other do not interfere [46, p. xxviii], [53, p. 37]. Correspondingly, T. Young (1773-1829) had hypothesized already in 1817 that light waves have to be transverse [46, p. xxviii], which fitted well into this picture.

Discovery of Fresnel equations.—In this situation, the polarization dependence of reflection and refraction had finally become a natural problem to study, and, astonishingly enough, it was solved very soon, in 1823, by A.-J. Fresnel [46, p. 42]. Fortunately, the equations now bearing his name could be corroborated almost immediately after their formulation by the ensuing theoretical derivation of the so-called Brewster angle, which had been discovered independently by D. Brewster (1781-1868) back in 1815 [47, p. 12].

We note that throughout all these developments, the index of refraction was defined by angular measurements. The first measurements of the speed of light in materials have only been performed by A. H. L. Fizeau (1819-1896), and later, A. A. Michelson (1852-1931) found agreement with refractive index measurements [54, p. 120].

3.2.2. Theory

Electromagnetic field theory.—Despite C. Huygens’ tentative derivation of refraction and reflection from field theoretical considerations [46, p. xxvi], by and large, the development of electromagnetic field theory went independently of the above experimental developments. The distinction between the fields $H$ and $B$ was introduced by W. Thomson (also: Lord Kelvin; 1824-1907) only in 1850. Later, these fields have been designated as “magnetic force” and “magnetic induction” by J. C. Maxwell (1831-1879) [55, p. 244], who successfully employed these concepts already in 1856 [56, p. 90]. The corresponding proportionality constant $\mu$ has been called “permeability” by W. Thomson [55, p. 245], after it had been introduced already in 1854 as
a “magnetization constant” by M. Faraday (1791-1867) [52, p. 547]. Moreover, Faraday already distinguished between para- and diamagnetism (see Refs. [57, p. 276] or [58, p. 401]). Similarly, the capacity enhancement by materials in a condenser was rediscovered—after unpublished results by H. Cavendish (1731-1810)—by Faraday in 1837, thus leading to the introduction of the “specific inductive capacity”, nowadays called permittivity or dielectric constant [59, p. 1]. Furthermore, Faraday already mentioned a state of “polarization” [58, pp. 327 f.]. By contrast, the so-called “displacement field” $D$ was only introduced by Maxwell in 1864 (see Refs. [58, p. 330] or [60]). This finally allowed for the definition of the permittivity as the ratio between the displacement field and the electric field [59, p. 1] in the sense of the equation $D = \varepsilon E$.

Maxwell relation.—In this situation, when both the electric permittivity, the magnetic permeability and the refractive index had been defined independently, Maxwell finally derived in 1865 an electromagnetic wave equation in materials with the wave velocity $v = c/\sqrt{\varepsilon_r \mu_r}$ [61, p. 104]. The corresponding formula for the refractive index, $n = \sqrt{\varepsilon_r \mu_r}$, can already be found in his original work, Ref. [62, Eq. (80)]. However, as it stood, the relation could not be verified with the data available at that time (see Refs. [63, vol. 2, p. 110] or [64, p. 142]). Astonishingly enough, the first tests were performed by Maxwell himself in 1871 for paraffin, but only approximate coincidence was found [63, vol. 2, p. 110]. Instead, it is L. E. Boltzmann (1844-1906) who is credited with the verification of the Maxwell relation in 1874 [57, p. 280]. While Faraday had still assumed that the dielectric constants of all gases coincide [52, p. 726], the differences in the permittivities of gases were first measured by E. W. von Siemens (1816-1892) in 1859 by means of a plate capacitor [52, p. 593]. Thus, in 1874 Boltzmann was in a position to verify the approximate relation $n^2 = \varepsilon_r$ for gases or, more generally, for those substances that do not display dispersion. In fact, many substances called “associating” at that time did not fulfill the Maxwell relation if the refractive index was measured at optical frequencies, while the dielectric constant could at best be measured independently at much lower frequencies (as is naturally the case with measurements relying on the plate capacitor). Fortunately, however, measurements of the refractive index at much lower frequencies became possible with the discovery of microwaves by H. R. Hertz (1857-1894) in 1886. Correspondingly, P. K. L. Drude (1863-1906) showed in 1897 that the “associating” substances (i.e., the substances showing dispersion) indeed also fulfill the approximate Maxwell relation $n^2 = \varepsilon_r$. 


at low frequencies \[59\], thereby requiring again the assumption that the relative magnetic permeability roughly equals one, i.e. \(\mu_r = 1\).

**Derivation of Fresnel equations.**—Finally, with the new field theory of electromagnetism, it remained to be shown that also the Fresnel equations could be recovered. Independently from the enquiry of the refractive index, whose standard formula \(n^2 = \varepsilon_r \mu_r\) had been taken for granted, this problem was solved by H. A. Lorentz (1853-1928). He rederived the Fresnel equations from Maxwell’s theory in 1875 in his doctoral thesis \[53\]. However, the derivation by Lorentz, which soon became standard, also required the assumption \(\mu_r = 1\) (see \(\S\)3.1). Interestingly, Lorentz later also introduced the distinction between microscopic and macroscopic electrodynamics \[65, 66\] and can therefore be considered the founding father of the Standard Approach to electrodynamics in media.

### 3.2.3. Conclusion

Fresnel’s equations are older than electromagnetic field theory. In fact, they have been derived independently of the Standard Approach to electrodynamics in media. Moreover, they have even been verified independently of this Standard Approach since, for example, the Brewster angle had already been discovered prior to Maxwell’s theory of electromagnetism.

In their original form of the “sine law” and the “tangent law”, Fresnel’s equations express the electromagnetic field amplitudes in terms of (incident and refracted) angles only (see Eqs. (2.7)–(2.10)). As such, these equations do not even require knowledge of the refractive index, the sole optical material parameter known at the time of their discovery. The refractive index on its side had already been known long since at that time. Therefore, the Fresnel equations constituted (and in fact still constitute) highly predictive statements, which as such would never have been accepted if they were not essentially true (with all possible “limitations” that any phenomenological law allows for). Furthermore, the Fresnel equations—be it in the form of the sine and tangent laws, or in the form involving the refractive index—hold independently of the latter’s relation to other material parameters such as the electric permittivity or the magnetic permeability. Thus, the Fresnel equations are extremely trustworthy and can even serve as a test case for any theoretical approach to electrodynamics in media.

By contrast, the picture is much more complicated when it comes to the Standard Approach to electrodynamics in media and its ensuing derivations of the refractive index and the Fresnel equations. In fact, when Maxwell
derived his formula for the refractive index, \( n^2 = \varepsilon_r \mu_r \), this was a predictive formula (at least in principle), because the material parameters \( \varepsilon_r \) and \( \mu_r \) had been defined (and partly even measured) independently of the refractive index. Unfortunately though, in the original interpretation where these electromagnetic material properties can be interpreted as capacity and inductance “enhancement factors”, the outcome of this formula is disastrous to say the least (take the example of water [45, Table 3.2]). In retrospect, this is not even surprising, as it had been clear already since Newton’s time that the refractive index depends on the frequency and can hence not be equal to frequency-independent material constants or products thereof (as the permittivity and permeability at Maxwell’s time really were).

Correspondingly, it became gradually clear to the scientific community that the standard formula—if it was to hold at all—should hold when all involved quantities refer to the same frequency. However, as direct measurements of the permittivity at optical frequencies are impossible even today, it appeared equally impossible to verify the standard formula as a matter of principle. Empirically, though, it turned out that for some substances (typically gases) the refractive index is roughly independent of the frequency, such that the standard relation for the refractive index could finally be verified in certain special cases by naively (so to speak, against the spirit of the equation) comparing the optical refractive index with the root of the static permittivity. For those substances whose dispersion could independently be established as weak, this comparison showed in fact a significant agreement. Later, it became even possible to verify the approximate Maxwell relation \( n^2(\omega) = \varepsilon_r(\omega) \) at low frequencies, where both the refractive index and the dielectric function could be measured independently (at the same frequency \( \omega \)). Curiously enough, this then somehow counted as a verification of the original Maxwell relation \( n^2 = \varepsilon_r \mu_r \), while in actual fact it had always been the approximate relation \( n^2 = \varepsilon_r \) which has been corroborated.

In addition, it must be emphasized that at optical frequencies, not even the relation \( n^2 = \varepsilon_r \) could ever be verified experimentally, since there the dielectric function turns out to be inaccessible. Instead, at optical frequencies, this formula is usually used as a defining equation which allows one to deduce the dielectric function from optical measurements. Fortunately, at present, the Maxwell relation obtains nevertheless a certain predictive power because the dielectric function can be calculated independently, namely by \textit{ab initio methods}. However, if the thus obtained dielectric function disagrees with the experiment, it is not clear whether this is due to the approximations inher-
ent in these ab initio methods or rather to a failure of the Maxwell relation used on the experimental side for determining the dielectric function. Correspondingly, the original equation \( n^2 = \varepsilon_r \mu_r \) becomes \textit{a fortiori} completely untestable in the optical régime, as this would require an independent measurement of \( n, \varepsilon_r \) and \( \mu_r \) at the same optical frequency.

In any case, in deducing the dielectric function from optical measurements, the Fresnel equations become instrumental as these allow for the determination of the refractive index in the first place. This is all the more noteworthy, since the derivation of the Fresnel equations from the Standard Approach even \textit{requires} the relation \( n^2 = \varepsilon_r \). By contrast, if the standard formula \( n^2 = \varepsilon_r \mu_r \) was true, then according to the Standard Approach, the Fresnel equations would have to be replaced by the pseudo-Fresnel equations \([3.25]–[3.28]\). These would not involve the refractive index but the wave impedance, and hence the dielectric function could not be deduced in the way it is usually done. Furthermore, Fresnel’s sine and tangent laws as well as the formula for the Brewster angle would not even be true in this case, as we will further explain in the next subsection.

3.3. \textit{Critique of standard derivation}

We have shown in §\[3.1\] that the Standard Approach to electrodynamics in media is not suitable for reproducing the Fresnel equations directly. Instead, the corresponding derivation ends up with Eqs. \([3.25]–[3.28]\) which we refer to as “pseudo-Fresnel equations”. As they stand, these equations differ grossly from the original Fresnel equations \([2.3]–[2.6]\) and the latter can only be recovered from the pseudo-Fresnel equations by means of the additional \textit{arbitrary assumption} (see the discussion in Ref. \[37\]) that \( \mu_r = 1 \) would hold for all materials (at least at optical frequencies). This assumption, which is apparently always introduced by sleight of hand, implies the Maxwell relation \( n^2 = \varepsilon_r \) and hence the equality of the inverse wave impedance and the refractive index. Correspondingly, sometimes already Eqs. \([3.25]–[3.28]\) are called “Fresnel equations”, which is, however, both factually and historically inaccurate.

We particularly stress that the allegedly more fundamental equation for the refractive index, \( n^2 = \varepsilon_r \mu_r \), is therefore \textit{not consistent with Fresnel’s equations}, as the latter can only be recovered from the Standard Approach if one assumes that \( \mu_r = 1 \) and consequently \( n = 1/Z = \sqrt{\varepsilon_r} \). On the other hand, if the arbitrary assumption \( \mu_r = 1 \) is dropped, then the pseudo-Fresnel
equations as derived in the Standard Approach actually contradict the independently established sine and tangent laws, Eqs. (2.8) and (2.10), as well as the formulae for the Brewster angle, Eq. (2.12), for the reflectance, Eq. (2.14), and for ellipsometric measurements of the dielectric function, Eq. (2.15).

However, an experimental deviation from these latter formulae—which could theoretically be accounted for by the introduction of a nontrivial magnetic permeability at optical frequencies—has apparently never been reported. We hence conclude that Eqs. (3.25)–(3.28) as derived from the Standard Approach have no experimental basis. In actual fact, those laws which have been verified experimentally are precisely the original Fresnel equations (2.3)–(2.6) and their ramifications (Brewster angle, reflectance formula, ellipsometry).

Astonishingly enough, this problematic state of affairs is not even restricted to the derivation of the Fresnel equations in the Standard Approach. Quite to the contrary, exactly the same problem is encountered already in the derivation of the refractive index itself: Here, the Standard Approach to electrodynamics in media leads to the equation \( n^2 = \varepsilon_r \mu_r \), while for practical purposes only the aforementioned approximation \( n^2 = \varepsilon_r \) is used. Precisely as in the case of the Fresnel equations, this is usually justified by the claim that \( \mu_r = 1 \) would hold at optical frequencies. Thus, in close parallel to the Fresnel equations, the original equation for the refractive index derived within the Standard Approach has no experimental basis. In fact, the considerations of §3.2 clearly show that it had been the experimental verification of the allegedly approximate relation \( n^2 = \varepsilon_r \), which in the first place led to the acceptance of Maxwell’s theory for the refractive index.

In view of this alarming absence of experimental confirmation, the authors of the present article have drawn in Ref. [37] the clearcut conclusion that the allegedly approximate relation \( n^2 = \varepsilon_r \) is actually the right formula for the refractive index, whereas the formula \( n^2 = \varepsilon_r \mu_r \) is plainly wrong and therefore lacking experimental evidence. Apart from a number of general arguments against the standard formula for the refractive index [37, §3.2], this conclusion had been confirmed independently by the direct rederivation of \( n^2 = \varepsilon_r \) from first principles [37, Sct. 4] within the Functional Approach to electrodynamics of media [34–41]. In the following, we will show that the same phenomenon arises when it comes to the Fresnel equations: a straightforward derivation within a microscopic approach to electrodynamics in media directly leads to the Fresnel equations (2.3)–(2.6) without the necessity of assuming \( \mu_r = 1 \).
4. Functional Approach

4.1. Introduction

We now come to the question of how the Fresnel equations can be reproduced within the framework of microscopic electrodynamics of media. For this purpose, we first note that the assumption $\mu_r = 1$ can already be introduced at the level of the boundary conditions (3.9)–(3.12) used in the Standard Approach. We then get the new boundary conditions

$$\mathbf{n} \cdot (\varepsilon_r \mathbf{E}_2 - \varepsilon_r \mathbf{E}_1) = 0,$$  \hspace{0.5cm} (4.1)

$$\mathbf{n} \times (\mathbf{E}_2 - \mathbf{E}_1) = 0,$$  \hspace{0.5cm} (4.2)

$$\mathbf{n} \cdot (\mathbf{B}_2 - \mathbf{B}_1) = 0,$$  \hspace{0.5cm} (4.3)

$$\mathbf{n} \times (\mathbf{B}_2 - \mathbf{B}_1) = 0.$$  \hspace{0.5cm} (4.4)

Since the Fresnel equations are obtained from the Standard Approach by setting $\mu_r = 1$ at the end of the derivation, one could alternatively perform the same calculation postulating $\mu_r = 1$ from the very outset, thus starting from the above boundary conditions (4.1)–(4.4).

Furthermore, as the representation of light rays by plane waves does not constitute a peculiarity of the Standard Approach, the problem of deriving the Fresnel equations in the Functional Approach actually simply boils down to the reproduction of the boundary conditions given by Eqs. (4.1)–(4.4).

In other words, if it can be shown that the Functional Approach directly leads to Eqs. (4.1)–(4.4) without setting $\mu_r = 1$, then the Fresnel equations (2.3)–(2.6) follow exactly in the same way as the pseudo-Fresnel equations (3.25)–(3.28) follow in the Standard Approach.

Thus, in order to derive the Fresnel equations within the Functional Approach, we only have to derive the boundary conditions (4.1)–(4.4). For this purpose, we first stress that the Functional Approach is a *microscopic* field theory which does away with the distinction between field theories “in matter” and “in vacuo”. Instead, within the Functional Approach all electromagnetic fields are determined by their respective Maxwell equations, whose form is independent of the presence of media. Therefore, if we want to describe refraction within the Functional Approach, we are confronted with different solutions of the microscopic Maxwell equations, which are restricted to different space regions (e.g., to an upper and a lower half-space in the case of a flat interface between two different materials). The question then simply
is: which conditions on these solutions can be deduced directly from the microscopic Maxwell equations? To this problem we now turn.

4.2. Microscopic boundary conditions

Given two solutions \( \{ \mathbf{E}_i, \mathbf{B}_i \} \) \((i = 1, 2)\) of the microscopic Maxwell equations with their respective sources \( \{ \rho_i, \mathbf{j}_i \} \), we consider the problem of whether these solutions can be “glued” together. By this, we mean the following: We single out a certain volume \( V \subset \mathbb{R}^3 \) and assume one solution to hold in its interior, while the other solution should hold in the exterior. In other words, we restrict the fields \( \{ \mathbf{E}_1, \mathbf{B}_1 \} \) to \( V \equiv \mathbb{R}^3 \setminus V \), and analogously for the sources. The question now is: are the resulting fields \( \{ \mathbf{E}, \mathbf{B} \} \), which are “glued” together from the individual solutions according to

\[
\mathbf{E}(x, t) := \chi_V(x) \mathbf{E}_1(x, t) + \chi_{\overline{V}}(x) \mathbf{E}_2(x, t), \tag{4.5}
\]

\[
\mathbf{B}(x, t) := \chi_V(x) \mathbf{B}_1(x, t) + \chi_{\overline{V}}(x) \mathbf{B}_2(x, t), \tag{4.6}
\]

again solutions of the Maxwell equations with appropriate sources? In these equations, \( \chi_V(x) \) denotes the characteristic function of the volume \( V \), i.e.,

\[
\chi_V(x) = \begin{cases} 
1 & \text{if } x \in V, \\
0 & \text{if } x \notin V,
\end{cases} \tag{4.7}
\]

while \( \chi_{\overline{V}}(x) = 1 - \chi_V(x) \) is the characteristic function of \( \overline{V} \).

To answer this question, we first note that the fields \( \{ \mathbf{E}_1, \mathbf{B}_1 \} \) and \( \{ \mathbf{E}_2, \mathbf{B}_2 \} \) separately fulfill the Maxwell equations in the interior of \( V \) and \( \overline{V} \), and hence the decisive point is only the behavior of the fields at the boundary \( \partial V \). Consider, for example, Gauss’ law. With the definition of the surface normal as

\[
n(x) := \nabla \chi_{\overline{V}}(x) = -\nabla \chi_V(x), \tag{4.8}
\]

we find from Eq. (4.5) that

\[
\nabla \cdot \mathbf{E}(x, t) = \frac{1}{\varepsilon_0} (\chi_V(x) \rho_1(x, t) + \chi_{\overline{V}}(x) \rho_2(x, t)) + \n(x) \cdot (\mathbf{E}_2(x, t) - \mathbf{E}_1(x, t)). \tag{4.9}
\]

Now, if we require the “glued” fields to fulfill again Maxwell’s equations, then the right-hand side of this equation must be interpreted as the corresponding
charge density $\rho(x,t)$ of the “glued” fields. This shows that an additional surface charge density $\rho_{\partial V}(x,t)$ arises, which is given by the last term in Eq. (4.9). This term is singular and not present in the original solutions of the Maxwell equations. Similarly, a straightforward calculation using the remaining Maxwell equations yields further conditions on the field behavior at the boundary, which we summarize as follows:

$$n \cdot (E_2 - E_1) = \rho_{\partial V}/\varepsilon_0,$$

$$n \times (E_2 - E_1) = 0,$$

$$n \cdot (B_2 - B_1) = 0,$$

$$n \times (B_2 - B_1) = \mu_0 j_{\partial V}.$$

This means, the “glued” fields given by Eqs. (4.5)-(4.6) indeed fulfill the microscopic Maxwell equations but with the following sources:

$$\rho(x,t) = \chi_V(x)\rho_1(x,t) + \chi_{\Gamma}(x)\rho_2(x,t) + \rho_{\partial V}(x,t),$$

$$j(x,t) = \chi_V(x)j_1(x,t) + \chi_{\Gamma}(x,t)j_2(x) + j_{\partial V}(x,t),$$

where the surface charge and current densities are given by

$$\rho_{\partial V}(x,t) = \varepsilon_0 n(x) \cdot (E_2(x,t) - E_1(x,t)),$$

$$j_{\partial V}(x,t) = \mu_0^{-1} n(x) \times (B_2(x,t) - B_1(x,t)).$$

The above formulae (4.10)-(4.13) constitute the general boundary conditions on the microscopic electromagnetic fields derived within the Functional Approach. (They may be compared with their counterparts in the Standard Approach given by Eqs. (3.1)-(3.4). In particular, Eqs. (4.10) and (4.13) are actually defining equations for the surface charge and current densities, whereas Eqs. (4.11) and (4.12) are necessary constraints, meaning that only such fields can be glued together which fulfill these equations. We further note that the general boundary conditions (4.10)-(4.13) follow directly from the microscopic Maxwell equations and therefore hold independently of the presence of media. The most important application, however, is given by the field behavior at the interface of different materials.

Before proceeding with the derivation of Fresnel’s equations in the next subsection, we perform a consistency check on the results obtained so far. In fact, we have shown that “gluing” together two solutions of the Maxwell
equations requires the introduction of new source fields given by Eqs. (4.14)–(4.15). Since the "glued" electric and magnetic fields satisfy the Maxwell equations with these new sources, the latter necessarily have to fulfill the continuity equation, i.e.,

\[ \partial_t \rho(x, t) + \nabla \cdot \mathbf{j}(x, t) = 0. \quad (4.18) \]

The reason for this is that the continuity equation can be deduced directly from the Maxwell equations (more precisely, from Gauss’ law and Ampère’s law with displacement current). As the consistency check, we now verify the above condition by an explicit calculation. First, the defining equations (4.14) and (4.15) imply that

\[ \partial_t \rho = \chi V \partial_t \rho_1 + \chi V \partial_t \rho_2 + \partial_t \rho_{\partial V}, \quad (4.19) \]

as well as

\[ \nabla \cdot \mathbf{j} = \chi V \nabla \cdot \mathbf{j}_1 + \chi V \nabla \cdot \mathbf{j}_2 + \mathbf{n} \cdot (\mathbf{j}_2 - \mathbf{j}_1) + \nabla \cdot \mathbf{j}_{\partial V}. \quad (4.20) \]

Using the respective continuity equations for the original sources terms,

\[ \partial_t \rho_i + \nabla \cdot \mathbf{j}_i = 0, \quad (4.21) \]

we then obtain the equality

\[ \partial_t \rho + \nabla \cdot \mathbf{j} = \partial_t \rho_{\partial V} + \mathbf{n} \cdot (\mathbf{j}_2 - \mathbf{j}_1) + \nabla \cdot \mathbf{j}_{\partial V}. \quad (4.22) \]

Now, the surface charge is given explicitly by Eq. (4.16), hence

\[ \partial_t \rho_{\partial V} = \varepsilon_0 \mathbf{n} \cdot (\partial_t \mathbf{E}_2 - \partial_t \mathbf{E}_1). \quad (4.23) \]

Similarly, we evaluate the divergence of the surface current using Eq. (4.17) and the vector identity

\[ \nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B}), \quad (4.24) \]

whereby we obtain

\[ \nabla \cdot \mathbf{j}_{\partial V} = \mu_0^{-1} \left( (\mathbf{B}_2 - \mathbf{B}_1) \cdot (\nabla \times \mathbf{n}) - \mathbf{n} \cdot (\nabla \times \mathbf{B}_2 - \nabla \times \mathbf{B}_1) \right). \quad (4.25) \]

On the other hand, with the vanishing rotation of gradient fields,

\[ \nabla \times \mathbf{n}(x) = \nabla \times (\nabla \chi V(x)) = 0, \quad (4.26) \]
and with Ampère’s law,
\[
\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \mu_0 \varepsilon_0 \partial_t \mathbf{E},
\]
Eq. (4.25) reverts to
\[
\nabla \cdot \mathbf{j}_{\partial V} = - \mathbf{n} \cdot \left( (\mathbf{j}_2 - \mathbf{j}_1) + \varepsilon_0 (\partial_t \mathbf{E}_2 - \partial_t \mathbf{E}_1) \right).
\]
Furthermore, by Eq. (4.23) this can be recast into
\[
\nabla \cdot \mathbf{j}_{\partial V} = - \mathbf{n} \cdot (\mathbf{j}_2 - \mathbf{j}_1) - \partial_t \rho_{\partial V}.
\]
Finally, plugging this formula into Eq. (4.22) yields the desired result, Eq. (4.18). Thus, we have shown that the introduction of the additional surface charges and currents given by Eqs. (4.16)–(4.17) is consistent with the continuity equation for the total sources.

4.3. Derivation of Fresnel equations

In the preceding subsection, we have derived the general boundary conditions on the microscopic electromagnetic fields, which are given by Eqs. (4.10)–(4.13). In this section, we come to the derivation of the approximate boundary conditions (4.1)–(4.4), which form the starting point for the derivation of the Fresnel equations. First, we see immediately that Eq. (4.11) coincides with Eq. (4.2) and Eq. (4.12) coincides with Eq. (4.3) anyway. Furthermore, Eq. (4.4) can be reproduced from Eq. (4.13) by setting the surface current to zero, as it is also assumed in the Standard Approach. It therefore only remains to derive the boundary condition (4.1) from the respective Eq. (4.10). For this purpose, we set again the surface current to zero, \( \mathbf{j}_{\partial V} = 0 \), as in the Standard Approach. By the continuity equation in the form of Eq. (4.29), this implies the additional condition
\[
- \partial_t \rho_{\partial V} = \mathbf{n} \cdot (\mathbf{j}_2 - \mathbf{j}_1).
\]
Now, with the definition of the surface charge density, Eq. (4.16) and with Ohm’s law in terms of the proper conductivity (see e.g. Ref. [37, § 2.5]), this translates into
\[
- \varepsilon_0 \mathbf{n} \cdot (\partial_t \mathbf{E}_2 - \partial_t \mathbf{E}_1) = \mathbf{n} \cdot (\tilde{\sigma}_2 \mathbf{E}_2 - \tilde{\sigma}_1 \mathbf{E}_1).
\]
By performing a Fourier transformation with respect to time, which implies the replacement \(-\partial_t \mathbf{E} \mapsto i\omega \mathbf{E}\), we obtain the equivalent formula

\[
\mathbf{n} \cdot \left( \left( 1 - \frac{\tilde{\sigma}_2(\omega)}{i\omega\varepsilon_0} \right) \mathbf{E}_2 - \left( 1 - \frac{\tilde{\sigma}_1(\omega)}{i\omega\varepsilon_0} \right) \mathbf{E}_1 \right) = 0.
\]  

(4.32)

Finally, substituting the proper conductivity in terms of the dielectric function by means of the standard relation (see Refs. [37, § 2.5] and [67])

\[
\varepsilon_{r,\text{eff}}(\omega) = 1 - \frac{\tilde{\sigma}(\omega)}{i\omega\varepsilon_0},
\]  

(4.33)

yields precisely the desired boundary condition (4.1). Thus, under the standard assumption of vanishing surface currents, we have derived the approximate boundary conditions (4.1) (4.4) which in turn correspond to the boundary conditions (3.9) (3.12) used in the Standard Approach for deriving the Fresnel equations. The point is, however, that the correct boundary condition (4.4) is automatically obtained in the Functional Approach, whereas the same equation follows only formally from the standard boundary condition (3.12) by setting \(\mu_r = 1\). Consequently, the Functional Approach also leads directly to the correct Fresnel equations (2.3) (2.6) without the detour of the pseudo-Fresnel equations (3.25) (3.28). This concludes our derivation of Fresnel’s equations from the Functional Approach.

5. Conclusion

We have subjected the standard derivation of Fresnel’s equations to a systematic critique, which is based on the following main arguments:

1. The Standard Approach to electrodynamics in media, which relies on the formula \(n = \sqrt{\varepsilon_r\mu_r}\) for the refractive index, does actually not reproduce the real Fresnel equations (2.3) (2.6) written terms of this refractive index. Instead, it leads to the “pseudo-Fresnel equations” (3.25) (3.28) in terms of the inverse wave impedance \(Z^{-1} = \sqrt{\varepsilon_r/\mu_r}\).

2. Only the real Fresnel equations (2.3) (2.6) imply the empirically verified “sine law” and “tangent law” as well as the formulae for the Brewster angle and for the deduction of the dielectric function from reflectivity and ellipsometric measurements (see Sct. 2).
3. Within the Standard Approach, this state of affairs can only be remedied by the arbitrary assumption \( \mu_r = 1 \), which implies the allegedly approximate relation \( n = \sqrt{\varepsilon_r} \). In particular, this arbitrary assumption also leads to the equality \( n = Z^{-1} \), by which the pseudo-Fresnel equations can be transformed into the real Fresnel equations.

4. It has been shown independently by the authors of this article that the allegedly exact formula \( n = \sqrt{\varepsilon_r \mu_r} \) is untenable [37]. Instead, within modern microscopic approaches to electrodynamics in media, one directly finds the formula \( n = \sqrt{\varepsilon_r} \) for the refractive index without the necessity of postulating \( \mu_r = 1 \) (see Ref. [37, § 4.4]).

5. Similarly, it has been shown in the present article that the Functional Approach to electrodynamics of media directly reproduces the original (i.e., real) Fresnel equations (2.3)–(2.6) without the detour of the pseudo-Fresnel equations (3.25)–(3.28).

Furthermore, we have derived the new, microscopic boundary conditions for the electromagnetic fields, Eqs. (4.10)–(4.13), which replace the older formulae (3.1)–(3.4) used in the Standard Approach. These new boundary conditions follow exclusively from the requirement that the electric and magnetic fields satisfy the microscopic Maxwell equations at the interface between two materials. Therefore, these new boundary conditions are not restricted to “macroscopically averaged fields”, and thus they are generally applicable in ab initio materials science.

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