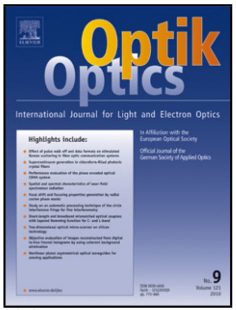

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Microscopic Theory of the Refractive Index

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Abstract

We examine the refractive index from the viewpoint of modern first-principles materials physics. We first argue that the standard formula, $n^2 = \varepsilon_{\mathrm{r}}\,\mu_{\mathrm{r}}$, is generally in conflict with fundamental principles on the microscopic level. Instead, it turns out that an allegedly approximate relation, $n^2 = \varepsilon_{\mathrm{r}}$, which is already being used for most practical purposes, can be justified theoretically at optical wavelengths. More generally, starting from the fundamental, Lorentz-covariant electromagnetic wave equation in materials as used in plasma physics, we rederive a well-known, three-dimensional form of the wave equation in materials and thereby clarify the connection between the covariant *fundamental response tensor* and the various cartesian tensors used to describe optical properties. Finally, we prove a general theorem by which the fundamental, covariant wave equation can be reformulated concisely in terms of the microscopic dielectric tensor.

Keywords: index of refraction, electrodynamics of media, ab initio materials physics

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1. Introduction

By the advent of first-principles materials science [1–4], the past decades have witnessed an unprecedented progress in the quantitative description of materials properties. Typical electromagnetic response properties, such as the conductivity and the dielectric tensor, are now within the reach of ab initio calculations [5–7], which thereby provide a new pathway to the theoretical design and optimization of functional materials [8–11]. A cornerstone in the development of first-principles electrodynamics of media has been the Modern Theory of Polarization [12–14], which first demonstrated the fallacy of simplified material models such as the Clausius-Mossotti picture of elementary electric or magnetic dipoles [15]. On the other hand, since such simplified models had played an important conceptual rôle in the Standard Approach to electrodynamics in media [16–18], the Modern Theory of Polarization also called for new perspectives on electrodynamics of materials which are based on first principles [19, 20].

Taking benefit of these ground-breaking insights, the Functional Approach to electrodynamics of materials has recently been developed by the authors of this article [21]. Its aim is the axiomatization and systematic elaboration of the already existing *microscopic* treatments of electrodynamics in materials as developed more or less independently in the electronic structure physics [22–24], semiconductor physics [25] and plasma physics [26] communities. The Functional Approach provides for a complete description of all linear electromagnetic materials properties in terms of the microscopic conductivity tensor (cf. [27–30]), a quantity which is routinely computed, for example, within the density functional theory framework [31–33]. In particular, this approach includes the formulation of *universal response relations*, which are analytical formulae suitable for the ab initio computation of all linear electromagnetic response functions. As the Functional Approach is exclusively based on the microscopic Maxwell equations, it is independent of a priori assumptions about the material, and therefore contributes to the modern pursuit of an unbiased first-principles description of materials properties.

The present article aims at contributing further to these developments by approaching also the optical properties of matter from first principles. The most important quantity in this context is of course the refractive index, by which the optical properties of many materials can be characterized [34]. The refractive index is usually defined as the ratio, $n = c/u$, between the speed of light in the vacuum and in the medium. In particular, it determines via Snell's law the reflection and refraction of light at the interface between two different materials [35, 36].

Ever since the foundation of classical electrodynamics by J. C. Maxwell in the nineteenth century, the standard formula for the refractive index,

$$n^2 = \varepsilon_{\mathrm{r}}\,\mu_{\mathrm{r}}\,, \tag{1.1}$$

has been a commonplace in almost all *theoretical* treatments of optics and classical electrodynamics [17, 18, 35–39]. It relates the refractive index n to the relative permittivity (or dielectric constant) ε_{r} and the relative permeability μ_{r} of the medium. For most *practical* purposes, however, the relative permeability does not play any rôle,

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